NSF-TIP Advanced Materials Opportunities

Contact: Gordon Long – glong@mitre.org

JSR-24-02

14 November 2024

Distribution A: Approved for public release. Distribution unlimited.

JASON
The MITRE Corporation
7515 Colshire Drive
McLean, Virginia 22102
(703) 983-6997

Contents

1 EXECUTIVE SUMMARY

The CHIPS and Science Act of 2022 authorized NSF to establish the TIP Directorate to “advance research and development, technology development, and related solutions to address United States societal, national, and geostrategic challenges, for the benefit of all Americans.” Included within the CHIPS and Science Act was an intent that the new TIP directorate enhance U.S. competitiveness via investment in translational research and development (R&D) in ten key technology areas. Within this list was “Advanced materials science, including composites, 2D materials, other next-generation materials, and related manufacturing technologies.” [1] While significant federal investment in fundamental research has led to the design and development of many new advanced materials as well as understanding of their fundamental properties, this new mandate is meant to expand innovation ecosystems both with regard to prior federallly funded research as well as a set of national challenges including national security and advanced manufacturing.

1.1 Statement of Work

JASON was asked by NSF to develop a set of specific technical investment hypotheses that NSF’s TIP Directorate could consider pursuing to increase U.S. competitiveness in one of the directorate’s key technology focus areas. The priority for JASON’s focus is to identify specific opportunities to accelerate the translation of research related to particular classes of advanced materials and/or advanced materials processing methods.

---

[1] `https://www.congress.gov/bill/117th-congress/house-bill/4346`

Specifically, JASON was asked to (Task list):

1. Identify particular classes of advanced materials and/or materials processing where:
    (a) past research investments have yielded extremely promising results;
    (b) applications have been identified and lab-scale proofs of concept have been conducted;
    (c) in spite of the foregoing, the research has not progressed further towards commercialization and/or only a limited degree of commercialization has been achieved;
    (d) and the JASONs determine through their study, especially through its qualitative and quantitative findings, that there is much greater potential that could be unlocked through near-term investments in research translation activities.
2. Identify a few compelling application / commercialization opportunities that could be enabled through advanced materials and/or materials processing. In contrast to the materials-up emphasis of the first task, this task would take an applications-down perspective.
3. Synthesizing the materials-up and applications-down perspectives, map out the rationale and modus operandi for compelling research translation investments. Emphasis should be placed on the next step(s) along the path to commercialization that TIP could undertake.
4. Attempt to identify 1-3 specific classes of materials in which AI/ML might play a very significant increased role in accelerating the creation of new materials with specific desired characteristics.

JASON received briefings from NSF and DoD on government perspectives, and representatives of academia and industry in four technical areas: critical materials, materials systems, microelectronics, and plastics and sustainability.

1.2 Key Findings and Recommendations

Based on these briefings and independent deliberations, JASON presents the following key findings and recommendations (F&R) first on the process by which NSF-TIP chooses opportunities for materials translation (Task 3 above) and then on each of three separate technical topic areas (Tasks 1-2 and 4 above). Additional findings and recommendations are included in the full text of the study.

The F&R in this section lay out the practical considerations for successful TIP programs in each area. In addition, for each of the translational materials opportunity hypotheses we have developed, we have identified specific materials/product examples which at present have the balance of "materials-up" push and "application-down" pull towards translation.

1.2.1 JASON's general findings and recommendations on the opportunities for TIP to accelerate the translation of materials to new technologies

These findings and recommendations are responsive to Task 3 regarding synthesis of the materials-down and applications-up perspectives to map out a general rationale for compelling materials research translational investments.

Findings:

F1 High impact translational opportunities for TIP investment in advanced materials are to be found in a "goldilocks zone" where there is both a *push* from a recent materials or materials system discovery *and a pull* from an existing or new application or technology space in which that material provides unique advantages and presents a value proposition.

F2 Common barriers prevent new materials and materials processing techniques from translating into new technologies. Many of these issues revolve around the difficulty in scaling up from the “bench-scale” science (gram scale) to the (multi) kilogram scale production of materials, a scale still far below the capacity of a pilot plant or manufacturing facility. This “development scale” highlights new challenges in materials synthesis, scale-up, and processing. The solutions to these challenges will require ongoing iteration with basic science leading to further innovation.

F3 Key approaches to overcome these common barriers to translation include:

a) Scaling up beyond lab-scale synthesis,

b) Early system-level integration of new materials,

c) Uniform testing and understanding of performance metrics, including durability and reliability,

d) Early inclusion of detailed technoeconomic and lifecycle analyses,

e) Engaging with industrial partners and government regulators.

F4 Accessible facilities that enable expansion beyond laboratory-scale experiments and models are essential for addressing scale-up challenges. These facilities amplify investments by engaging more researchers than can be directly funded, enhancing uniformity in testing and materials reliability, and broadening workforce development, but must include industrial participants both in planning stages and as users to assure relevance to future translation.

F5 AI/ML could play a substantial, increased role in accelerating the creation of new materials with specific desired characteristics. Rather than mapping such opportunities to ”specific classes of materials”, JASON believes that the opportunities need to leverage and are critically dependent on gathering and analyzing large-scale data of basic materials properties, details of processing and manufacturing, as well as performance within the final applications. Although details of AI/ML will differ according to material and application, the collection and calibration of such data will be facilitated by:

(a) Collaborations with existing national user facilities,
(b) Establishing specialized user facilities as needed for specific materials problems,
(c) Instrumented automation of experiments and scale-up,
(d) Capturing, labeling, and categorizing large amounts of curated process data,
(e) Uniformity in testing and characterization,
(f) Working with industrial experts able to help define and populate relevant data bases.

Recommendations:

R1 NSF-TIP should focus on materials maturity, defined by value proposition, scalability, durability, and reliability, in identifying materials systems that are compelling research translation investments.

R2 NSF-TIP funding should focus on addressing the "beyond-lab-scale" barriers to translating materials into new technologies. This includes scaling materials production from grams (laboratory scale) to the 10 kg scale and supporting necessary iterations with basic science to bridge material development toward significant applications. Specific examples with respect to each of the investment opportunities are discussed within the text of the report.

R3 In parallel with direct R&D investments, NSF-TIP should consider funding independent facilities relevant to different materials and application areas to address common barriers to materials translation. These facilities should be established with data generation/curation and AI/ML training in mind, following best practices for uniform data handling to enable future use in AI/ML models and training.

R4 NSF-TIP advanced materials programs should be implemented with focused data generation/curation and potential AI/ML training in mind. TIP should provide each program with sufficient resources to both use and develop realistically-sized and effective data bases related to the materials goals of the program.[2]

R5 NSF-TIP should establish strong and diverse relationships with the entities that fund the basic science materials discovery efforts that will ultimately push translation. These include the NSF Division of Materials Research and Engineering Directorates as well as other agencies including the National Institute of Standards and Technology.

---

[2] We will amplify specific opportunities for AI/ML in the focus areas of Thermal Management for Semiconductor Packaging and Alternatives to Fluorinated Materials.

R6 Given the mandate within the CHIPS and Science Act to develop translational research and development efforts that benefit national and economic security [3], we recommend NSF-TIP establish strong relationships and communication with entities likely to *pull* new innovations. These include the Department of Defense, regulatory agencies such as the Environmental Protection Agency, the national security community, and a broad base of industrial representatives in materials technologies.

1.2.2 JASON's findings and recommendations on translational opportunities for a circular economy for plastics

Recent years have seen significant development of new lab-scale chemical routes towards managing plastic waste many of which show significant promise. As a result, there is now a "materials-up" opportunity (Task 1), or *push* to translate these discoveries into practice resulting in the continual regeneration and re-use of plastics. In this case, barriers to translation and opportunities for TIP to bridge center primarily around understanding whether and how these lab-scale discoveries translate into larger scale processes and realistic feedstocks.

Findings:

F6 Significant federal and industrial funding has led to the development of numerous possible routes towards a circular economy for rarely recycled commodity polymers including polyolefins, polystyrene, and polyvinyl chloride including inventions ranging from new catalysts for chemical recycling to new biomass-derived alternative materials. So far, commercialization and large scale demonstrations have been limited.

---

[3] `https://www.congress.gov/bill/117th-congress/house-bill/4346`

F7 Life cycle analysis (LCA), encompassing materials, energy and water costs, environmental impacts, and technoeconomic analysis (TEA), encompassing a true comparison to the cost of existing technologies, are critical to a compelling value proposition. The LCA and TEA estimations improve as science and process design mature.

F8 Laboratory experiments are performed at small scale on pure materials, while full-scale production requires integration with accepted processing techniques for less ideal polymers. Similarly, biomass processing experiments at the lab scale use a single feedstock, but accurate LCA and TEA estimations require the use of realistic feedstocks and appropriately scaled synthesis and processing.

F9 Scale-up from a round bottom flask or a Parr reactor in a laboratory to process-scale equipment handling highly viscous polymer melts is an iterative process that both presents new challenges as well as inspires new scientific directions. This iterative process is not generally pursued via basic science programs in polymer science and the lack of iterative understanding, as well as the lack of universal rules to scale-up to larger process equipment and production rates, are major barriers towards the translation of new polymer recycling solutions.

Recommendations

R7 NSF-TIP should make investments in translation of plastics waste recycling specifically for the large scale consumer polyolefins (polypropylene and polyethylene), polyvinyl chloride, and polystyrene where *development scale* experiments and iterative scale-up are critical to success.

R8 NSF-TIP should support iterative process development of recycling solutions based on recent scientific breakthroughs in polymer chemical recycling, specifically, development of techniques and catalysts compatible with large scale processing of plastics likely to advance breakthroughs towards translation. Further, development of catalysts that are tolerant to the impurities and additives in commodity polymers will occur iteratively as experiments proceed at the development scale.

R9 Ensure that LCA and TEA are completed in-pace with iterative scale-up processes to give realistic feedback on the viability of plastic circularity solutions and to inspire problem solving.

1.2.3 Findings and recommendations on thermal management systems for semiconductor packaging

For current advanced microelectronics systems, the high power densities of the component chips, as well as multi-chip integration, mandates new approaches to thermal management of packaged systems. This area constitutes a major "applications-down" (Task 2) opportunity for TIP. While research has identified new thermal management materials and cooling approaches, modeling will be needed to anticipate coupled thermal-electrical-mechanical effects. As is true for plastics, the barriers to translation and opportunities for TIP relate to bringing simple thermal management solutions into larger-scale processes under controlled, repetitive fabrication conditions. Thermal management solutions could benefit from accurate systems-level modeling; advancement in this area could be significantly accelerated via the use of AI/ML if appropriate data on which to train the models are collected (Task 4).

Findings:

F10 Advances in modern high-performance electronics depend on more than scaling to smaller feature sizes and higher densities. Innovative 2.5D and 3D device architectures composed of multiple chips and chiplets, e.g., Heterogeneously Integrated (HI) Systems in a Package (SiP), will be critical for future advanced computing and signal processing. These architectures will require new materials solutions for thermal management and packaging.

F11 Advanced microelectronics systems (such as HI in SiPs) exacerbate challenges in thermal management, offering opportunities for new materials and material systems solutions. Thermal effects in such HI systems are strongly coupled to electrical and mechanical performance, and materials solutions for these “Thermal Interface Materials” (TIMs) must also accommodate these constraints.

F12 Modeling and simulation are crucial for directing materials choices and strategic testing for the thermal performance of high-performance heterogeneous integrated systems. Modeling tools need to be extended to cover the full range of length scales and include thermal-electrical-mechanical effects across the numerous interfaces in these systems. Additionally, simulations must consider details of how HI systems are assembled, such as the methods of material deposition.

F13 AI and ML can improve the quality of modeling and simulation and reduce the design cycle time in this area, but only with an extensive, well-catalogued, and curated database of necessary materials and process parameters along with system-level performance data. Data collection should be explicitly structured to enable the investigation and quantification of process-structure-property relationships through AI/ML.

Recommendations:

R10 NSF TIP should fund research projects that model, process, and evaluate proposed TIMs and heat spreader technologies within a systems context. This will lay the foundations for a better long-term match between research innovation in and industrial adoption of advanced materials for microelectronics.

R11 NSF TIP, in partnership with other areas of NSF and other organizations funding basic research, should fund the development of multi-scale, multi-physics systems-level models for thermal management in HI systems, including coupled thermal-electrical-mechanical effects.

R12 NSF TIP should leverage and expand existing facilities to pilot multi-level, multi-property SiP testing for the research community, establishing well-calibrated procedures for such testing.

R13 NSF TIP should partner with other relevant government agencies to create pilot facilities for simple, but well controlled and monitored, integrated processing for HI microelectronics thermal management. These pilot facilities should collect and curate processing-related and systems-level performance data, which will enable AI/ML -facilitated system-level thermal, electrical, and mechanical models supportive of new materials integration.

1.2.4 Findings and Recommendation on Alternative Materials for PFAS

Following recent and somewhat sudden changes to both regulations and market drivers in the Spring of 2024, alternatives to fluorinated materials have emerged as a critical need across a number of industries as well as national and economic security interests. While significant recent and historical scientific work in PFAS alternatives exists, the rapidity of the changes in the market make this a key "application-down" opportunity for TIP (Task 2). In addition, the potential use of historical data in the structure-function relationship of PFAS alternatives also suggests that this is a key area where AI/ML, powered by properly curated databases, may be able to signficantly enhance translation (Task 4).

Findings:

F14 PFAS supplies are likely to be constrained by market contractions and reduced domestic production. While replacements are emerging for consumer products, essential uses in industry, semiconductors, and national security are at risk, making these PFAS products *critical materials*.

F15 In the prior decades of research and development, a vast amount of data, much of it proprietary to industry, has been amassed on the properties and synthesis of PFAS materials, as well as alternative materials that have been considered for similar functions. While much of this may be soon leveraged for near-term solutions, in some application cases, the Carbon-Fluorine bond in PFAS may be irreplaceable because, for example, it imparts extraordinary temperature and chemical stability.

F16 The essential use concept[4] as well as the American Innovation and Manufacturing Act (AIM) allow continued use of essential products if use of a replacement substance is impossible or impractical. However, these provisions cannot protect even essential uses from

---

[4] `https://www.whitehouse.gov/wp-content/uploads/2023/03/OSTP-March-2023-PFAS-Report.pdf`

market constrictions that result in a loss of domestic availability of products. The domestic availability is of particular importance to national security applications.

F17 Several methods for alternatives to fluoropolymers or for alternative fluoropolymer manufacturing are being developed to reduce environmental leaching. Transitions to these alternatives will likely focus on large markets with less demanding requirements. Consequently, the DoD may struggle to find manufacturers for specialty versions needed for their essential use applications including binders for explosives and o-rings for demanding environments.

F18 The already-existing vast amount of industrial data on the properties and synthesis of PFAS materials and alternative materials can constitute a substantial and highly-leveraged data base for AI approaches that may be able to reduce time-to-translation of PFAS alternatives.

Recommendations:

R14 NSF-TIP should focus efforts on PFAS replacements that are critical to economic security, e.g., fluorine-free photo-acid generators for lithography in the microelectronics industry, and national security, e.g., DoD-specific applications, with particular attention to drop-in alternative materials to minimize disruption in essential uses.

R15 For irreplaceable fluorinated materials in essential applications, NSF-TIP should prioritize translation of manufacturing and processing methods, with highest priority on eliminating environmental release, e.g., synthesis and manufacture of fluoropolymers that do not contain leachable fluorinated small molecule surfactants.

R16 NSF TIP should support the transition away from PFAS by implementing expanded Materials Genome[5] R&D concepts under the AI Aspiration for Sustainable Materials[6]. This includes developing databases of structural, physical, and functional properties, as well as training data for processing procedures.

---

[5] https://www.mgi.gov

[6] `https://ai.gov/wp-content/uploads/2024/06/AIA-Materials-0624.pdf`

2 INTRODUCTION

2.1 Historical Perspective on NSF Technology, Innovation, and Partnerships (TIP) Directorate

The CHIPS and Science Act of 2022 authorized NSF to establish the TIP Directorate to "advance research and development, technology development, and related solutions to address United States societal, national, and geostrategic challenges, for the benefit of all Americans." Included within the CHIPS and Science Act was an intent that the new TIP directorate enhance U.S. competitiveness via investment in translational research and development (R&D) in 10 key technology areas. Recognizing the constraints of current and projected budgets, NSF recently published a TIP Roadmap [82] to guide a staged investment strategy. That strategy focuses on a subset of the key technology areas, and lists a set of three core objectives:

1. Cultivate diverse innovation ecosystems throughout the U.S. to advance use-inspired research and innovation in key technologies and to address societal and economic challenges;
2. Advance U.S. competitiveness in critical and emerging technologies by developing and translating innovations and addressing national challenges;
3. Grow a diverse and inclusive next-generation talent base and workforce around key technology and challenge areas, building expertise in necessary technical skills, use-inspired research and innovation, entrepreneurship, and translation.

One of the originally-identified key technology areas related to "Advanced materials science, including composites, 2D materials, other next-generation materials, and related manufacturing technologies.” While significant federal investment in fundamental research in advanced materials has advanced understanding, this new mandate is meant to expand innovation ecosystems both with regard to prior NSF investments as well as those of specific mission requirements including defense and energy.

2.2 Objectives of this study

Our objective was to develop a set of specific technical investment hypotheses that NSF’s TIP Directorate could consider pursuing to increase U.S. competitiveness in this key technology focus area. The priority for JASON focus would be on advanced materials, to identify specific opportunities to accelerate the translation of research related to particular classes of advanced materials and/or advanced materials processing.

Specifically, JASON was asked to (redacted quotations from the Statement of Work):

1. Identify particular classes of advanced materials and/or materials processing where: (i) past research investments have yielded extremely promising results; (ii) applications have been identified and lab-scale proofs of concept have been conducted; (iii) in spite of the foregoing, the research has not progressed further towards commercialization and/or only a limited degree of commercialization has been achieved; (iv) and JASON determines through the study, especially its qualitative and quantitative findings, that there is much greater potential that could be unlocked through near-term investments in research translation activities.
2. Identify a few compelling application / commercialization

opportunities that could be enabled through advanced materials and/or materials processing. In contrast to the materials-up emphasis of the first task, this task would take an applications-down perspective.

3. Synthesizing the materials-up and applications-down perspectives, map out the rationale and modus operandi for 3-5 compelling research translation investments. Emphasis should be placed on the next step(s) along the path to commercialization that TIP could undertake (and could reasonably afford to undertake).
4. Attempt to identify 1-3 specific classes of materials in which AI/ML might play a very significant increased role in accelerating the creation of new materials with specific desired characteristics.

2.3 The Process of Translation of Materials Innovation to Practice

In the process of materials design and discovery (early stages of materials maturity), synthesis, processing, and characterization of materials are done at a relatively small lab-bench scale. Translation towards incorporation within a technology requires not only an understanding of properties and scalability that may not be obvious at this stage, but also depends on the ability to integrate the new material within an existing framework and trust that it will perform reliably over timescales frequently far beyond that of a laboratory experiment. This constitutes a major barrier for the translation of new materials: the technology designer or entire industry must trust the performance promise of the new material. Trust in this context equates to the body of knowledge available for the material that quantifies all the relevant properties in the proposed application. Trust also depends on accumulated experience with successful use of the material in terms of consistent properties and absence of failures under standard operating conditions.

It is also commonly the case that actual materials are not monolithic pieces incorporated into a structure (e.g. a fuselage skin) but rather entire integrated systems in which the materials interactions and interfaces are ideally net positive as opposed to detractive (e.g. an integrated chipset with thermal management system). Importantly, a new material is commonly more expensive than those that it may replace and there is a colloquial phrase that it has to "buy its way into the application," meaning that there has to be a business case that the improved performance and/or reliability justifies the extra cost. Alternatively, a shifting societal or regulatory framework may alter the value proposition for a new material set or processing framework (e.g. sustainability and circularity). The role of simulation is important because it is increasingly used to predict the properties and guide the synthesis effort for new materials. As confidence in a material builds, there is also a need for simulating the processing steps although this is considered to be more challenging. JASON previously developed a Materials Maturity Levels concept [33] to address this need for a very high level of materials maturity prior to potential incorporation into a technology.

Finding 2.1: Technology integration requires that materials demonstrate a value proposition (economic, life cycle, regulatory) and be scalable, reliable, and durable.

Recommendation 2.1: NSF-TIP should focus on materials maturity as defined by value proposition, scalability, durability, and reliability in identifying materials systems that are compelling research translation investments. (**R1**) [7]

---

[7] designation **R1** indicates this is a Key Finding or Recommendation included in the Executive Summary of this report

2.4 JASON Rationale

The current research and development (R&D) environment includes activities in both new materials design as well as the application of materials to new and existing technologies, which are not always matched. Indeed, while materials discovery activities regularly introduce new classes of materials with interesting properties, providing a *push* for new materials, an important signpost of readiness for potentially impactful translational investment is a clear *pull* from a technology or industry for which this new material (with almost necessarily higher initial cost) is uniquely suited. Sections 6-8 will details exemplar areas that JASON believes fit within this zone between *push* and *pull*.

Finding 2.2: High impact translational opportunities for TIP investment in advanced materials are to be found in a “goldilocks zone” where there is both a *push* from a recent materials or materials system discovery and a *pull* from an existing or new application or technology space in which that material provides unique advantages and presents a value proposition. (**F1**)

From our briefings from industrial leaders, academic experts, and funding agencies (listed in Appendix B) and our study of materials investment opportunities, we sought to identify exemplar classes of advanced materials or system applications that were in the “goldilocks zone” of demonstrated maturity from many perspectives, yet lacking specific demonstrated realizations to spur industrial applications. In this context, we recommend investments in the following topics, which will be further expanded upon in the remainder of the report.

Recommendation 2.2: NSF-TIP should consider a set of exemplar areas which satisfy a “goldilocks zone” of materials maturity in terms of translational readiness.

Section 6: A Circular Economy for Plastics

Section 7: Thermal and Packaging Challenges in Electronic Systems

Section 8: Replacement of Fluorinated Compounds in Formulations and Materials for Semiconductors and Energetics

Within the context of our briefings, we heard several examples of materials with exciting properties that we chose not to include in our recommendations because the timing did not seem ideal for an NSF-TIP translational investment (not yet in the "goldilocks zone"). For illustrative purposes, we will give examples of a few of these materials classes and point to some signposts that would indicate to NSF-TIP a readiness for investment and provide greater detail in Section 9:

2D materials serve as a useful example of a class of promising materials that were not included in our initial and exemplar set because they appeared to require a more clear application *pull* to provoke translation. From briefings organized by NSF for JASON on the subject, we concluded that: Graphenes are an older class of 2D materials which have provoked great excitement due to the unique properties of the materials within a single sheet, but have found limited application space beyond niche heat sinks and sports products largely due to an inability to scale their impressive electronic and other properties beyond the size of a single sheet. To provide a broader context, in 2013 the European Commission (EC) started the *Graphene Flagship*, a research and innovation program with a budget of 1 billion Euros. This project ran for ten years and provided funding to a consortium of approximately 170 academic and industrial partners spanning 22 countries and collaborating on the development of marketable products containing graphene and related 2D materials [28]. The program was founded on the promise of numerous application pulls, and included 20 million Euros funding of a 2D Experimental Pilot Line (2D-EPL). A few commercial applications are only beginning to emerge [35]. MXenes are a newer class of 2D inorganic materials that exhibit remarkable and perhaps unique tunability in terms of structure, elemental composition, and surface terminations that impart properties ranging from high conductivity to important optical and redox properties as well as durability. Unlike graphenes, the properties of MXenes are retained in thin films with overlapping individual flakes. However, as stated in [53], "...the 2D materials are close to market. But will they find their killer app?" From the JASON perspective, translational investment is only meaningful if an application *pull* already exists.

Recommendation 2.3: 2-D materials ranging from graphene to MXenes have impressive properties but a unique *pull* towards a specific application or technology was not yet clear to us. There continue to be exciting developments, particularly in MXenes so we recommend a periodic survey of application or technology *pull*.

Ceramics and composites are useful examples of materials and supporting disciplines with significant historic maturity. In the briefings organized by NSF for JASON, we heard interesting vignettes regarding what is still not understood about the role of interfaces with respect to both thermal barrier materials and structural materials within these categories. In this context, translational opportunities in advanced materials generally arise from basic science investments leading to discoveries of new materials design paradigms and even new classes of materials. These categories of materials have seen this kind of investment in recent years within the context of DOD thermal barrier coatings and other similar applications, but not in a manner that leads to broader *push* of translational opportunities.

Recommendation 2.4: Ceramics and composites are important materials for national security and energy applications such as thermal barrier coatings. Outside of this already substantially funded context, we did not find discoveries that would provide a strong *push* towards translation based on new materials design paradigms or discoveries. We recommend observation for strong *pushes* towards translation in areas in which investments will not be swamped by existing investments by DOD.

In Section 9 we explore several materials systems that we found exciting either for reasons of recent materials innovation *push* or because of strong societal/technological *pull* but we deemed to be not yet ready for a major translational investment. In each case we both present signposts of readiness and some suggestions for ways in which TIP could also help advance readiness.

2.5 Advanced Materials in the NSF-TIP Context

TIP has already initiated a variety of programs that span the key technology areas outlined in the CHIPS and Science Act including Advanced Materials. We list some of the most relevant of these programs below as these investments are likely highly complementary to the programs recommended in this report that focus specifically on Advanced Materials.

2.5.1 TIP's Convergence Accelerator Program

JASON commends the innovations represented by TIP's Convergence Accelerator Programs to encourage team-based approaches in delivering high-impact solutions meeting societal needs. The recently announced Phase 2 awards [8] in Sustainable Materials have relevance and areas of overlap with the topics discussed in this report. For example,

---

[8] `https://www.nsf.gov/awardsearch/advancedSearchResult?ProgEleCode=131Y00&BooleanElement=Any&BooleanRef=Any&ActiveAwards=true#results`

- **FUTUR-IC** “aspires to address the major bottleneck to the continued scaling of microchip performance at constant cost, power, and improved environmental footprint, with a STEM and green-innovation-trained workforce, by pioneering pathways for the heterogeneous integration of processor, accelerator, and memory chips within a common package, and by creating new electronic-photonic integration technologies.“
- **PFACTS** led by IBM Corporation “will accelerate efforts to replace, redesign and remediate fluorine-containing per- and polyfluoroalkyl substances (PFAS), or ‘forever chemicals,’ used in many products and processes such as non-stick coatings, compostable food containers and semiconductor manufacturing. The PFACTS knowledge base and artificial intelligence tools enable stakeholders to assess PFAS hazards, prioritize replacements and identify remediation materials to find faster solutions for forever chemicals.”
- **Topological Electric** intends to accelerate topological materials toward low cost next-generation energy and information devices with environmental sustainability, scalability and superior performance. The project will develop electronic and energy harvesting device prototypes based on topological materials.

The Accelerator Program’s required “idea-to-market” curriculum cultivates an entrepreneurial and product mindset and should lay the groundwork for future success in translation of foundational work in materials into the marketplace. NSF has advised that “By the end of Phase 2 (3 years), teams are expected to provide deliverables that impact societal needs at scale and are sustainable beyond NSF support.”

JASON’s recommendations seek to identify complementary resources that TIP might provide to translate materials capabilities into needed applications. Some of these recommendations may apply to multi-scale, systems-level modeling that has relevance to a broad range of materials systems. Some recommendations may relate to the development of facilities that can provide pilot-scale exploration of materials and systems scale-up, or trusted calibrations of materials properties.

2.6 Conclusion

JASON appreciated the opportunity to collaborate with NSF and others on this important topic. The remaining sections of the report detail JASON's investigation into translational opportunities in advanced materials:

- Section 2 discusses the process of translation of materials innovations to practice within the NSF-TIP context.
- Section 3 includes a discussion of the common barriers to materials translation.
- Section 4 discusses the physical barriers to materials translation in terms of facilities and access to *development scale* experiments.
- Section 5 expands on opportunities for artificial intelligence (AI) and machine learning (ML) to accelerate translation as well as the converse: opportunities for the process of materials translation to provide curated data to train future AI/ML models.
- Sections 6, 7, and 8 in turn discuss specific opportunities in A Circular Economy for Plastics, Thermal and Packaging Challenges in Electronic Systems, and Alternatives for Fluorinated Materials.
- Section 9 includes some shorter vignettes on those materials opportunities which we do not recommend for high priority at this time with some "lessons learned" about translational opportunities.

- Section 10 contains our concluding remarks and thoughts for future opportunities.

This Page Intentionally Left Blank

3 COMMON BARRIERS TO MATERIALS TRANSLATION

Our list of materials translational opportunities (Sections 6-9) is exemplary of current opportunities as identified through the lens of JASON expertise. In this context, we also identify several common "valleys of death" that must be overcome to achieve high materials maturity and technology advancement. We observe that these common issues appear to be agnostic of materials category and apply to most application or technology sectors, *e.g.,* the defense sector [16]. As a result, we suggest that NSF-TIP focus on these barriers within any translational effort in advanced materials. Further, we identify that several of these issues are best solved via the combination of R&D funding as well as the establishment of national user facilities at a scale and with a technical uniformity not typical of academia. These national user facilities will also serve to integrate a broader base of researchers, industrial experts, and future workforce than a single R&D effort.

3.1 Common Valleys of Death in Materials Translation

The phrase "valley of death" is used commonly to refer to the challenge of advancing innovations in research-based ideas and materials to commercialization, i.e., overcoming barriers to technology translation. Typically, it is necessary that there exists a technology *push*, in the form of existing science and engineering understanding and demonstrated experimental plausibility of an idea. At the same time, it is important that there is an industrial *pull*, i.e., a demonstrated need for a solution that is economically competitive, perhaps taking into account government action to achieve societally responsible actions, e.g., clean air and water, food and energy security, etc.

Translation, almost by its very nature, requires iteration between the science and engineering that first suggested an advance and the results that are achieved when a commercial application is attempted. This iterative theme is particularly true when materials processing, materials integration, and scale-up are needed to move beyond laboratory scales.

On the positive side, the very nature of a valley of death means that it acts as a filter to eliminate poorly conceived ideas/approaches. We focus on the former: how to best approach the challenge of moving beyond a laboratory idea to what is often a somewhat messier, less controlled, environment that accompanies carrying through to commercialization.

It should not be forgotten that typically it takes significant time to advance from an idea to a successful process and product. For example, the float (or flat) glass process, which is used for a large fraction of glass and window products in the world, was introduced in the 1950s. It is a continuous flow process that ensures reliability, high quality, and productivity and does so at a low production cost [46]. The modern approach was introduced by Pilkington in 1952, and, once it was perfected, revolutionized the production of flat glass, and in turn the uses of flat glass products. How long was that effort? According to Pilkington Company History, it took seven years and more than 7 million pounds (more than 100 million USD in today's money) to develop the full process [46].

Similarly, decades of materials research resulted in the availability of light emitting diodes (LEDs) of different colors starting in the early 1960s, and red LEDs rapidly found commercial applications for small displays and numeric indicators. It was early realized that blue LEDs, combined with existing red and yellow LEDs had the potential to create white lighting with low heat dissipation. Several researchers made progress in growth of

GaN materials as early as the late 1960s, but the lack of suitable templates for the growth, and the poor quality of the materials were daunting [30]. However, materials breakthroughs (the scientific *push*) between 1986 and 1993 showed the possibility of LEDs and lasers formed on GaN-materials, an important precursor to the first commercially available “white light” LED lightbulbs. It was important that the new breakthroughs focused not only on the materials properties, but also developed the necessary device-level materials doping and contacts.

Also important was the possibility of a strong market and policy driven *pull* for LED lighting. This was achieved by careful consideration of policy incentives to adopt an initially unknown and more expensive lighting source. The Energy Policy Act of 2005 (EPACT 2005) and the Energy Independence and Security Act of 2007 (EISA 2007) issued directives to the Secretary of Energy to carry out a Next Generation Lighting Initiative to support Solid State Lighting (SSL) research, development, demonstration, and commercial application activities. For nearly two decades, the DOE Solid-State Lighting Program [71] has brought together researchers, industry, universities, standards organizations, utilities, energy efficiency programs, building owners, lighting designers, and specifiers to drive SSL technology advances, ensuring that researchers address critical issues in LED efficiency improvements within a broader ecosystem that addressed manufacturability, cost, and market acceptance. An important incentive to SSL development may also have been the rapid adoption and marketing of this technology by China [47]. Worldwide market share of LED lighting is expected to keep increasing to about 75 percent by 2025 and near total market saturation in the 2030s [73].

3.1.1 Advice to address materials-specific valleys of death

Since the valleys-of-death challenge is well known, there is a literature addressing the topic, from business and technical aspects. Materials specific themes appropriate to the Department of Defense are discussed in a 2004 NRC report [48]. Here we offer a few guidelines, inspired by [16], that may assist program directors in identifying and managing projects with the goal to achieve successful translation. In particular,

> Theme 1: Is it worth the effort?
>
> > Does the new technology's intended use address a compelling materials need?
>
> Theme 2: Is there an adequate potential commercial market?
>
> > Is the science and engineering support compelling and does it address a market need?
>
> Theme 3: Is there an industry partner that can develop the technology effectively and efficiently?
>
> > Can the technology be manufactured easily and at a competitive price?

There are distinct issues to be overcome, each that goes beyond the laboratory-scale materials research that was likely the first step in the process. They include

(a) Scale-up: An important step is to produce quantities at scales large enough for the intended application, which is generally significantly larger than feasible in the laboratory. This challenge is well known in industry and often requires iteration with the research team to adjust the conditions so as to process either larger quantities while maintaining the same quality, or produce faster, or both.

(b) Uniform testing and establishment of performance metrics that are relevant to the application – data compared and analyzed across different research groups and contributors.

(c) Testing and understanding of durability and reliability.

(d) Early inclusion of detailed technoeconomic and lifecycle analysis based on the target application.

(e) Any issues that industrial partners must address with government regulators, e.g., safety or health.

3.1.2 Existing NSF programs recognizing the valleys of death

NSF has recognized for many years the challenge posed by the valleys of death in advancing fundamental science and engineering supported by NSF to impact industry (see list in Appendix D). One relatively recent example is the Partnerships for Innovation (PFI) program, which has in its description [76]:

> "PFI has five broad goals, as set forth by the American Innovation and Competitiveness Act of 2017 ('the Act', S.3084 — 114th Congress; Sec. 602. Translational Research Grants):
>
> (1) identifying and supporting NSF-sponsored research and technologies that have the potential for accelerated commercialization;
>
> (2) supporting prior or current NSF-sponsored investigators, institutions of higher education, and non-profit organizations that partner with an institution of higher education in undertaking proof-of-concept work, including the development

> of technology prototypes that are derived from NSF-sponsored research and have potential market value;
>
> (3) promoting sustainable partnerships between NSF-funded institutions, industry, and other organizations within academia and the private sector with the purpose of accelerating the transfer of technology;
>
> (4) developing multi-disciplinary innovation ecosystems which involve and are responsive to the specific needs of academia and industry;
>
> (5) providing professional development, mentoring, and advice in entrepreneurship, project management, and technology and business development to innovators.
>
> In addition, PFI responds to the mandate set by Congress in Section 601(c)(3) of the Act (Follow-on Grants), to support prototype or proof-of-concept development work by participants with innovations that because of the early stage of development are not eligible to participate in a Small Business Innovation Research Program or a Small Business Technology Transfer Program.
>
> Finally, PFI seeks to implement the mandate set by Congress in Section 102(c)(a) of the Act (Broader Impacts Review Criterion Update) by enhancing partnerships between academia and industry in the United States, and expanding the participation of women and individuals from underrepresented groups in innovation, technology translation, and entrepreneurship."

PFI has been moved to the TIP Directorate. In addition, on July 31, 2024 (as this report was being written), NSF-TIP announced the first Assessing and Predicting Technology Outcomes (APTO) investments with the goal of ascertaining the "specific science and technology investments that will enable the nation to intentionally accelerate the development of key technologies that are essential to long-term national security and economic prosperity [79].”

Finding 3.1: Common barriers prevent new materials and materials processing techniques from translating into new technologies. Particularly challenging are issues associated with scaling up from the gram scale typical of bench-top work in academic labs to the multi-kilogram scale needed for development of materials prior to further scale-up in a pilot plant or manufacturing facility. This “development scale” highlights new challenges in materials synthesis, scale-up, and processing. The solutions to these challenges are iterative with basic science and lead to further innovation. (**F2**)

Finding 3.2: Key approaches to counter these common barriers to translation include (**F3**):

a) Scaling up beyond lab-scale synthesis
b) Early system-level integration of new materials
c) Uniform testing and understanding of performance metrics, including durability and reliability
d) Early inclusion of detailed technoeconomic and lifecycle analyses
e) Engaging with industrial partners and government regulators

Recommendation 3.1: NSF-TIP funding should focus on addressing the “beyond-lab-scale” barriers to translating materials into new technologies. This includes scaling materials production from bench-scale (subgram to gram-scale, depending on materials category) to development scale (kilogram and greater, depending on the application) and supporting necessary iterations with basic science to bridge material development toward significant applications (**R2**).

Recommendation 3.2: NSF-TIP should establish strong and diverse relationships with the entities that fund the basic science materials discovery efforts that will ultimately push translation. These include the NSF Division of Materials Research and Engineering Directorates as well as other agencies including the National Institute of Standards and Technology (**R5**).

Recommendation 3.3: Given the mandate within the CHIPS and Science Act to develop translational research and development efforts that benefit national and economic security [9], we recommend NSF-TIP establish strong relationships and communication with entities likely to *pull* new innovations. These include the Department of Defense, regulatory agencies such as the Environmental Protection Agency, the national security community, and a broad base of industrial representatives in materials technologies (**R6**).

---

[9] `https://www.congress.gov/bill/117th-congress/house-bill/4346`

4 FACILITIES THAT ENABLE MATERIALS TRANSLATION

The preceding discussion about common barriers to materials translation raises several specific issues. One major barrier has to do with the physical scale at which materials are made: materials discovery is done at the benchtop scale with quantities that may be as small as micrograms or as large as grams. Integrating (as opposed to designing) a new material into an existing process, application or system [66] requires much larger quantities of order tens of grams up to tens of kilograms depending on the materials class, which we discuss below in section 4.1. The facilities to accomplish such scaleup are few in number and hard (if not impossible) for materials developers to access. Collaboration between materials designers (the "push") and industry users ("the pull") is essential not just for scale-up but also for training and developing the workforce, including, in the case of students, the future workforce.

Finding 4.1: Accessible facilities that enable expansion beyond laboratory-scale experiments and models are essential for addressing scale-up challenges. These facilities amplify investments by engaging more researchers than can be directly funded, enhancing uniformity in testing and materials reliability, and broadening workforce development. (**F4**)

Recommendation 4.1: In parallel with direct R&D investments, NSF-TIP should consider funding independent facilities relevant to different materials and application areas to address common barriers to materials translation. These facilities should be established with data generation/curation and AI/ML training in mind, following best practices for uniform data handling to enable future use in AI/ML models and training (**R3**).

The methodologies used in bench-scale proof of concept experiments differ so greatly from those used in manufacturing scale that the facilities alone present a barrier to translation. For example, in an academic laboratory, a student may process a small batch (<1 gram) of a polymer blend via solution blending or small scale compounding to measure its properties whereas large scale manufacture will be done using a twin screw extruder and other process equipment. Further, the successful manufacture of materials requires extensive "know-how" which is regarded as vital or proprietary information whether it be in a research lab or in industry. Patents on materials commonly describe composition and final state along with proposed applications but rarely describe the processing, which is often held as a trade secret.

4.1 Scale-up to Development Scale – Synthesis and Processing

Lab or bench-scale research and development is generally done on a relatively small scale for reasons of efficiency, cost, and safety. The latter is particularly true in academic environments, typically funded by NSF, and where the researchers are trainees. This trend is true across all disciplines of materials science though the definition of *small* varies. Unfortunately this presents a series of challenges towards translation as creating a strong value proposition for the new material generally requires more than this *small* scale amount of material. We will term this intermediate range the *development scale* as it enables the following:

1. Equipment and operations occurring at small scale are frequently not directly scalable. Simply put: Solutions that work at small scale do not necessarily scale volumetrically to larger scale. For example: in terms of mixing, a magnetic stir-bar on a hot plate is

sufficient at the 100 mL scale but not at the kilogram scale, much less at industrial-reactor scale.

2. When larger scale equipment and methods are introduced, fundamental aspects of the science change. For example, the method of mixing causes different shear fields, which may be damaging to the catalysts used or the materials themselves, inspiring new scientific insights and developments. These new insights have the potential to dramatically change the technoeconomic and life cycle analysis thereby changing the value proposition.
3. Frequently, *development scales* of material are required to measure material properties, reproducibility, and durability.

Unfortunately, due to both the safety issues and the inherent expense, a single academic laboratory is unlikely to have sufficient equipment or personnel to perform the critical development scale experiments delineated above. While industry has production scale equipment available, this is not generally available for redirection as it is engaged in earning a return on the capital invested *i.e.,* a *return on investment* (ROI). Machines engaged in production are highly constrained to meet specifications of the purchasers. Those specifications are often considerably tighter in terms of process or operation parameters than given by the publicly available datasheet (or relevant patent).

Consequently, development and integration of a new material, even where the composition is not too different from an existing alloy (for metallics), represents a substantial investment of time and effort to develop the production know-how, even if the same machinery can be used. Moreover, given the uncertain prospects of the quantities that might be sold, the ROI is likely to be inadequate. The developer of the material is very unlikely to have all the machinery required, which leads to an impassable valley of death in terms of new material translation. One of the authors of this report had precisely this experience when seeking a source of weld wire (for use in directed energy deposition, DED, additive manufacturing) in a particular titanium alloy. None of the very small number of companies that manufactures such wires would consider a contract to supply the wire even if the feedstock were supplied to them.

Large-scale facilities funded by NSF, Department of Defense, and the Department of Energy exist for basic materials science synthesis and characterization (lab or bench scale), but rarely cross over into this critical development scale. The NSF National Nanotechnology Coordinated Infrastructure (NNCI) has enabled major discoveries, innovations, and contributions to education and commerce via open accesses university user facilities in the general area of nanofabrication primarily at the laboratory scale with limited opportunities for exploring the development and manufacturing scales.

Some examples of existing facilities with the capability of performing *development scale* processing of metallics exist in certain national laboratories, notably the Sigma facility at the Los Alamos National Laboratory and the Powder Synthesis and Development Capability at the Ames National Laboratory. The latter has a nearly unique capability for making metal powders and is known for its advancements in gas atomization. The Sigma facility processes a very wide range of metals and ceramics for diverse programs. However, the facility carries high overhead related to its security, and other protocols associated with its largely defense-oriented mission tend to prevent substantial use by academic researchers.

The DoD ManTech program supports LIFT – Learning Innovations For Tomorrow – “develops and deploys new advanced materials manufacturing technologies and processes, including lightweighting and multi-material processing in support of our national economy and national defense.” This facility has broad capabilities relevant to structural materials but, again, focuses on defense needs.

4.1.1 Current status of testing and characterization facilities

The U.S. government supports a wealth of facilities for materials characterization and testing funded by NSF, DOE, DoD, DOC (NIST), and NASA in addition to facilities in the commercial sector. The NSF facilities that support advanced materials testing and characterization include those funded as small-scale (*e.g.,* NSF Major Research Instrumentation grants (NSF-MRI)), mid-scale instrumentation grants (NSF Mid-scale Research Infrastructure-1 (Mid-scale RI-1)), and large-scale centers (NSF Major Multi-user Facilities *e.g.,* The National High Magnetic Field Laboratory (NHMFL) and Cornell High Energy Synchrotron Source (CHESS) all essentially dedicated to furthering basic science through the NSF-DMR division.

DOE has a network of national user facilities for basic and applied science that is the envy of the world[10], almost all of which focus on academic laboratory-scale samples. These facilities include synchrotron sources and beamlines, neutron scattering sources and instruments, large optical and free-electron laser facilities, electron microscopy centers, and nanoscience centers and instruments. Existing NSF directorates have established partnerships with these facilities that include funding operations, supporting instruments, and user support including operators, academic faculty, and (importantly) students for workforce development.

Uniform testing and characterization for scale-up to production differ strongly in concept and execution from characterization of academic laboratory scale samples in capturing processing data. Recent advances in laboratory automation and robotics are likely to enhance both

---

[10] `https://www.energy.gov/science/office-science-user-facilities`

consistency in processing and the ability to vary and capture process parameters across controlled ranges within the testing scheme [21]. There are thus opportunities for TIP to create and fund similar partnerships at existing facilities that will enable translation science that are distinct from current basic and applied science programs at these facilities. TIP could support the creation of dedicated mid-scale facilities (*e.g.,* beamlines at current synchrotron sources) dedicated to testing and characterization that currently do not exist. A notable trend at user facilities is an increase in data quantity (e.g., from higher resolution detectors) and data rate (higher fluxes of neutrons and x-rays combined with more efficient detector read-out). The user facility managers and operators are aware of the challenges and the need for faster data reduction, [11]. While higher throughput and quality of data are enabling of materials discovery efforts, these facilities are almost exclusively aimed at research as opposed to translation.

A different kind of partnering could occur with DoD, for example with the Manufacturing Innovation Institutes (MIIs, https://www.dodmantech.mil/About-Us/Manufacturing-Innovation-Institutes-MIIs/), which have a similar translation mission but one limited to defense needs (JSR- 23-03). There may also be a need for altogether new facilities that do not exist within the current ecosystem of NSF, DOE, DoD, DOC, and NASA facilities to support the TIP mission. This would necessarily include instruments and facilities needed for qualification of materials, components, and devices as part of scale up through the valley of death toward large-scale production. These needs will differ with respect to the materials systems being studied and will therefore need to closely parallel NSF-TIP research investments to enable accelerated translation.

---

[11] https://www.alcf.anl.gov/news/argonne- researchers-pioneer-new-approach-automating-data-processing-workflows

Another distinguishing feature of TIP-supported dedicated advanced materials facilities would be an emphasis on critical role for partnerships with the commercial sector. This should include, in particular, an opportunity for startup companies that lack sufficiently sophisticated facilities for characterization and testing that they need to bridge their own valleys of death to large-scale production.

This Page Intentionally Left Blank

5 DATA CAPTURE FOR ACCELERATED DEVELOPMENT AND ML/AI TRAINING

It is nearly a truism to state that accelerated materials discovery, processing, and scale up can only proceed with substantial, well-structured databases. To be useful for advanced materials applications, data sets must cover the full parameter space of the problem to be addressed. This may lead to unmanageably large data bases, or proliferation of multiple data sets that cannot be interconnected, unless criteria for expandability are built into the database structure from the beginning.

Just in the past few years, publicly available datasets relevant to materials analysis have proliferated in any given area, including public, searchable forums such as Mendeley Data. Indeed, there are examples of data-aware materials discovery such as novel high-temperature materials and battery materials [44, 87]. These are mostly focused on relationships between composition and properties with limited information on processing, *e.g.,* a heat treatment. Large datasets such as those from the Materials Project [67] tend to be focused on a single specific static property and do not include processing information such as mixing, phase separation, interdiffusion, interfacial interactions, and decomposition. For most materials areas, microstructure-properties datasets exist but processing-relevant microstructure-properties datasets are rare. As a result, JASON's general recommendations on AI/ML acceleration of materials translation focus primarily on the need for relevant data with which to train models. Specific recommendations on materials in which AI/ML tools could accelerate translation are included in Sections 7 and 8.

5.1 Data Requirements

Advanced Materials development requires databases designed for processing information in addition to typical properties data. Database design may also differentiate between optimization across a limited range of variables, and discovery, which will require much broader exploration. More than that, the push-pull Goldilocks zone that we advocate for TIP investment involves combining materials into emulsions, mixed solids, components, and systems of components. Here, the relevant data include both static and dynamic properties of the interactions between materials, including the interfaces between components as well as the interfaces within (e.g., heterogeneous or composite) materials that play a key role in determining system-level properties and performance. Examples include (all with temperature dependence) surface energies, viscosities, mechanical properties, diffusion, and conductance (chemical, thermal, electrical); friction and other tribological properties; and dissipative responses, all of which are sensitive to materials details, such as the presence and distribution of impurities, defects, and interfaces.

The need to cover such a wide range of parameter space highlights the need for automated data acquisition over systematically controlled ranges of parameter variations. This approach is well recognized in the literature [29], and automation is likely to enhance both consistency in processing and the ability to vary and capture process parameters across controlled ranges within the testing scheme [21]. There is strong interest in use of such data, but growth in approaches that actually implement experimental measurement and application of physical and process information has been relatively slow [44, 87]. The sheer size of the parameter space for complex materials properties, compounded by the wide range of processing conditions, can become a barrier to implementing the experiments needed. While we strongly endorse the FAIR (Findable, Accessible, Interoperable, and Repeatable) principles described in the next sub-section, they should not be taken as a prescription to develop “perfect” databases in competition with advancing materials development. The two can and should be carried out in parallel with iterative development of the best data base components and practices along with demonstrating successful new processing pathways.

Finally, we explicitly address the utility of AI/ML for accelerating advanced materials development. There is ample reason to believe that AI/ML could assist, perhaps uniquely, in accelerated deployment of complex materials and materials systems. That accelerated development and deployment can play a critical role in facilitating the translation of materials into commercial applications. Early examples include connecting properties to microstructure where the methods are often drawn from advanced statistics (as opposed to deep learning): another example relates to Tang *et al.* [64] demonstrating how scraping all the available literature data allowed a new index for hot cracking susceptibility to be developed. Moving from this point to achieving high impact results will only happen if there is sufficient training data to map out the processing-to-properties connection. An early win in beginning to develop such data bases may come through close collaboration with industrial materials suppliers. Future materials and processing methods will build on previous experience with producing useful materials, most of which is in the industrial sector. To build on this knowledge base, TIP should establish strong partnerships with industrial teams interested in using data analytics and AI/ML to reduce the timescale for discovering new materials and bringing the to market.

5.2 FAIR Principles for Structured Data Sets

To be useful, materials data must be consistently well organized across time and groups. The FAIR (Findable, Accessible, Interoperable, Repeatable) principles define the requirements for data at a high level [86]. Enabling these attributes imposes substantial additional requirements: a filename convention must agreed upon, preferably constructed so as to make the source of the data self-describing; a sample ID system must be agreed upon which allows for tracking of the subdivision of bodies of material during the characterization process. While this kind of nomenclature is well established in some materials categories, in others (e.g. polymers) the advent of a universally accepted structurally based identifier (representation) system and data structure has been a major challenge [41][83].

Applications nearly always require a specialized set of properties to be measured to a depth that permits statistical analysis as a prelude to building confidence in that material. Characterization and testing is costly in terms of labor. For example, in structural materials, a rough hierarchy even for microstructure (a relatively straightforward task) starts with visual inspection, then optical microscopy, then scanning electron microscopy with a plethora of branches into texture, orientation scanning, Raman microscopy, atomic force microscopy, etc. Testing for properties in these kinds of materials may start with basic tensile tests and proceed to variable temperature, strain rate, stress relaxation, rheometry, etc. Other vital properties such as corrosion, creep (low strain rate), or fatigue are slow to execute and therefore more costly but often cannot be avoided for qualifying a material for a given application. In other materials that may be used across a wide variety of application spaces, this range of relevant structures and properties becomes even broader. For example, poly(ethylene oxide)-based materials are widely used for everything from batteries (as a solid electrolyte) to cosmetics and biomedical applications.

The FAIR attributes also have consequences in terms of the necessity for descriptions of the characterization and/or test parameters, *i.e.,* recording the meta-data along with the data themselves. If the team involved in the *development scale* synthesis, scale-up and processing facility for, say, recycling a particular plastic is to exchange data between groups for the purposes of applying AI/ML to build a process-structure-properties model, each side of the exchange must reach an agreement about the structure of said data. This has been discussed in the literature (*e.g.,* Ghiringhelli *et al.* [25]), but standards are few and far between for good reason, which is that each research area has widely varying needs for characterization and testing, as outlined above. Finally, preserving datasets over long periods of time comes with a cost; thus any facility or center that is stood up to tackle a specific materials translation must organize its approach to data from the inception. This task becomes all the more challenging when testing is done on an academic scale across a large heterogeneous sampling of materials and characterization tools resulting in a wide variety of data sets in disparate locations.

Finding 5.1: AI/ML could play a substantial, increased role in accelerating the creation of new materials with specific desired characteristics. Rather than mapping such opportunities to "specific classes of materials," JASON believes that the opportunities need to leverage and are critically dependent on gathering and analyzing large-scale data of basic materials properties, details of processing and manufacturing, as well as performance within the final applications. Although details of AI/ML will differ according to material and application, the collection and calibration of such data will be facilitated by (**F5**):

(a) Collaborations with existing national user facilities
(b) Establishing specialized user facilities as needed for specific materials problems
(c) Instrumented automation of experiments and scale-up
(d) Capturing, labeling, and categorizing large amounts of curated process data

(e) Uniformity in testing and characterization

(f) Working with industrial experts able to help define and populate relevant data bases

Recommendation 5.1: NSF-TIP advanced materials programs should be implemented with focused data generation/curation and potential AI/ML training in mind. TIP should provide each program with sufficient resources to both use and develop realistically-sized and effective data bases related to the materials goals of the program. Specific opportunities for AI/ML will be amplified in the focus areas of Thermal Management for Semiconductor Packaging and Alternatives to Fluorinated Materials in this report. (**R4**)

6 A CIRCULAR ECONOMY FOR PLASTICS

The 20th and 21st centuries have seen modern life revolutionized by the introduction of lightweight, strong, easily disinfected plastics. The extremely low cost of this class of materials led to a perception of infinite disposability and a global economy and culture built around single-use plastics. As a result, the amount of plastic waste generated globally more than doubled from 2000 to 2019, reaching 353 Mt (million tons) per year[52]. Clearly, recycling plastic waste would have societal benefits, but the process of mechanical recycling results in significant material property degradation at an expense and energy cost sometimes higher than the production of the raw materials. This results in a very limited incentive to recycle plastics; only between 9-15% is collected for recycling and even less is actually recycled. The rest is either incinerated, dumped in landfills, or leaked from the waste management system entirely to the detriment of sensitive ecosystems and human health, as shown in Figure 6-1.

This lack of circularity presents a major environmental threat both with regards to landfills and aquatic environments, which constitutes a regulatory and consumer-driven *pull* for this opportunity. Significant industrial and academic funding has resulted in scientific solutions ranging from a new generation of catalysts that breakdown polymers to small molecules that are of higher value and new biomass-derived plastics, constituting a major new innovation *push* towards translation. While these scientific breakthroughs continue to progress at the laboratory and demonstration scales, NSF-TIP has an opportunity to help translate alternative circularity solutions from the lab to the development scale where major questions remain regarding the strength and durability of new plastics and the efficiency, robustness, and reliability of new chemical recyclng solutions. *This is suggested as a major "materials-up" opportunity for translation for NSF-TIP (Task 1).*

6.1 A Need for Translation and Scale-up

NSF-TIP has a significant opportunity to impact the circularity of plastics use by leveraging recent breakthroughs across academia, government laboratories, and industry in the fundamental science of polymer recycling and biodegradation towards industrial translation. Over the past decade, significant federal funding has enabled the advancement of new scientific materials concepts ranging from the synthesis of biomass derived polymers to catalysts that enable chemical recycling.[12]. In particular, numerous new catalysts (some of these are highlighted in Appendix E) have been discovered that allow extraordinarily stable commodity plastics to be efficiently degraded to higher value chemicals[62][36][85]. Translation beyond the laboratory scale demonstration will require an iterative process where scale-up efforts will shed light on unforseen scientific challenges that must be addressed, as illustrated in Figure 6-2. This iterative scale-up barrier is common amongst many new materials systems at the translation stage, but is particularly pertinent in the problem of polymer waste management whose scale is on the order of millions of tons/year. Translation requires not only funding for beyond lab-scale experimentation and system-level process-focused computation, but also interactions with industry and government to develop a waste handling and regulatory framework for implementation.

Finding 6.1: Significant federal and industrial funding has led to the

---

[12] `https://www.nsf.gov/news/news_summ.jsp?cntn_id=303230&org=EFMA&from=news`, `https://www.nsf.gov/awardsearch/showAward?AWD_ID=2317582`, `https://csp.umn.edu/`

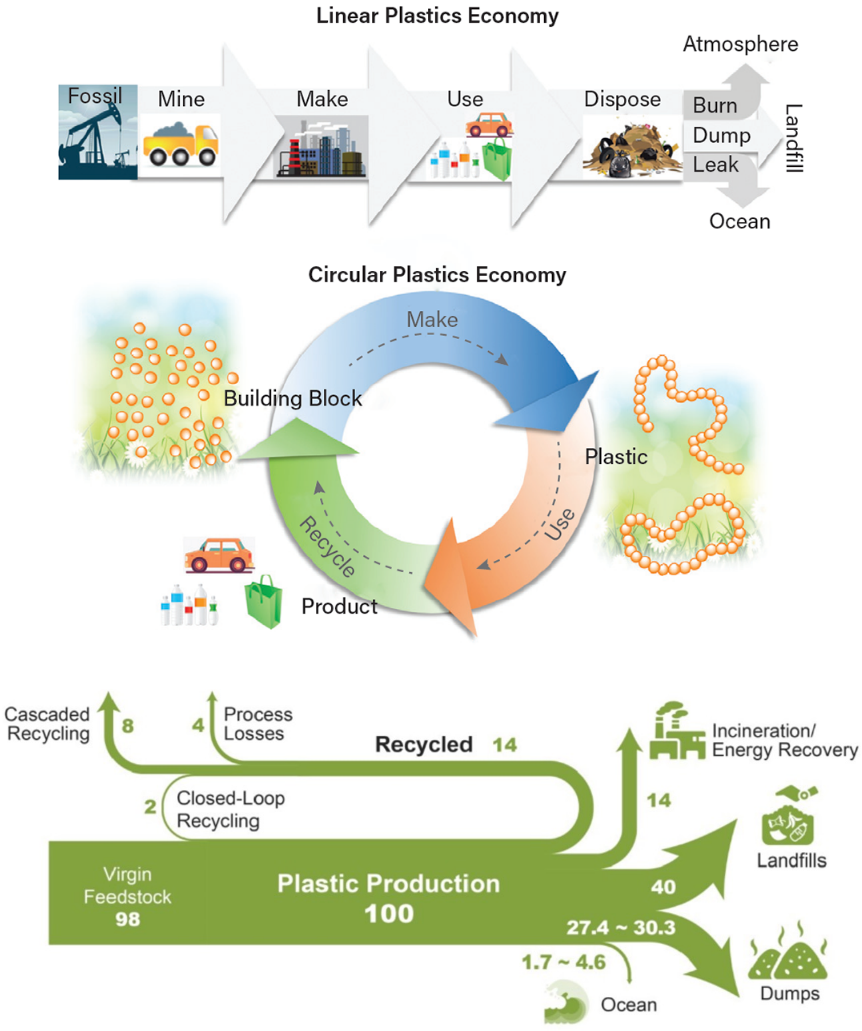


Figure 6-1: A circular plastics economy would return all plastics back to building blocks from which new materials could be made [8]. This is a paradigm shift from the current situation (bottom Sankey Diagram) showing that a minimal amount of current plastics production relies on closed-loop recycling [40].

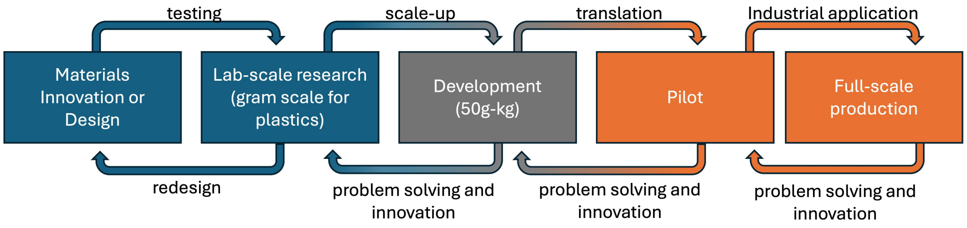


Figure 6-2: The process of translation from a materials design to industrial practice, particularly in commodity plastics requires multiple phases of scale-up towards an ability to test designs and then scale-down to solve problems. Each circular loop results in additional innovation and invention. Both blue boxes are within a typical basic science project involving reactions and processes on the gram (or sub-gram) scale. The two orange boxes (pilot and full-scale production facilities) are generally completed within industry. Translation, however, is predicated on the demonstration of features (e.g., strength maintained across several recycle scales, synthesis within a continuous process as opposed to a lab-scale reactor) requiring scale-up towards a development scale on the order of 50 g - 1 kg batches (gray box) rarely accomplished in materials innovations originating from academic environments.

development of numerous possible routes towards a circular economy for plastics use and enabled inventions ranging from new catalysts for chemical recycling to new biomass derived materials. So far, commercialization has been limited to relatively small start-up-scale efforts (**F6**).

Recommendation 6.1: NSF-TIP should make investments in translation of plastics waste recycling specifically for the large scale consumer polyolefins (*e.g.,*polypropylenes and polyethylenes), polyvinyl chloride, and polystyrene where *development scale* experiments and iterative scale-up are critical to success (**R7**).

Finding 6.2: Laboratory experiments are performed at small scale on pure materials, while full-scale production requires integration with accepted processing techniques for less ideal polymers. Similarly, biomass processing experiments at the lab scale use a single feedstock, but accurate life-cycle analyses (LCA) and technoeconomic analyses (TEA) require the use of realistic feedstocks and appropriately scaled synthesis and processing (**F8**).

Finding 6.3: Scale-up from a round bottom flask or a Parr reactor in a laboratory to process-scale equipment handling highly viscous polymer melts is an iterative process that presents new challenges but can also inspire new scientific directions. This iterative process is not generally pursued via basic science programs in polymer science and the lack of iterative understanding, as well as the lack of universal rules to scale-up to larger process equipment and production rates, are major barriers towards the translation of new polymer recycling solutions (**F9**).

Recommendation 6.2: NSF-TIP should support iterative process development of recycling solutions based on recent scientific breakthroughs in polymer chemical recycling, specifically, development of techniques and catalysts compatible with large scale processing of plastics likely to advance breakthroughs towards translation. Further, development of catalysts that are tolerant to the impurities and additives in commodity polymers will occur iteratively as experiments proceed at the development scale (**R8**).

6.2 Strategies Towards a Circular Plastic Economy

Unlike glass and aluminum recycling, consumable plastics are actually a broad class of different chemistries presenting challenges associated with separation as well as unique requirements with respect to processing and recycling in each individual case, as shown in Figure 6-1. Further, within each class, a wide variety of chemical additives are included in consumer plastics including stabilizers, plasticizers, impact modifiers, pigments, and flame retardants. Current recycling methods require an expensive and time consuming task of separating and sorting the wide variety of plastic wastes – resulting in a situation where, with current regulations, it is frequently cheaper and easier to simply make a new plastic product rather than recycle.

Over recent years, three major strategies have emerged to improve the circularity of plastics:

1. Mechanical Recycling, which refers to the reuse of a previously processed or waste material in the same chemical format.
2. Chemical Recycling via the catalytic, enzymatic, or solvent-based conversion of polymers to small molecules
3. Bioplastics from renewable resources that are frequently biodegradable.

As an example of the possible routes to recycling, poly(ethylene terephthalate) (PET) is the most recycled commodity plastic; 31% is recycled in the US, and Europe and Japan recycle substantially more. It is the only plastic that is currently both mechanically and chemically recycled and has the potential for biodegradation. As shown in Figure 6-3, mechanical recycling of PET is predicated on numerous sorting and separation steps followed by several mechanical processing steps that have the unfortunate side effect of breaking down the chains and degrading mechanical properties. For this reason, though mechanical recycling is currently the most commonly implemented approach, it is not "closed-loop". As a result $< 1\%$ of plastics are mechanically recycled more than once. Here, PET is at a unique advantage: the ester linkages in its backbone allow for post-recycling reactions to extend the chains and rectify the damage done by mechanical recycling [54]. This ability to heal the bonds after the damage caused by reprocessing is part of why PET alone is very highly recylced via mechancial routes. For this reason, there is little incentive to find alternatives to mechanical recycling of PET, though it often serves as a good testbed for the development of chemical or biological recycling routes. Numerous publications have focused on the biodegradation via exposure to a PET-digesting enzyme originally discovered to be be excreted by *Ideonella sakaiensis* 201-F6 [90]. While these are academically exciting, implementation of biodegradation routes on PET is unlikely to be of tremendous translational impact given the current ability to efficiently recycle this chemical route. Similar biodegradation routes for other plastics (specifically polyolefins) are much farther from the *goldilocks zone* in terms of technological readiness. Similarly, PET's ester groups can be hydrolyzed at high temperatures to produce the constituent monomers, enabling chemical recycling. These monomers are more easily purified than the plastic and can then be repolymerized to make a new "virgin" PET in a completely virtuous circularity cycle [60]. Nevertheless, chemical recycling of PET is not commercially implemented due to its relatively high energy cost [11, 15].

6.2.1 Development of scalability in chemical recycling approaches

The remaining 5 ASTM-coded plastics experience significant molecular weight and property degradation upon mechanical recycling and also cannot currently be chemically recycled due to the strength of the carbon-carbon bond. Moreover, they have no known route towards biodegradation. All have been the subject of significant federally funded efforts including large consortia or academic collaborations such as the NSF-CCI: Center for Sustainable Polymer Science at the University of Minnesota and the BOTTLE (Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment) Consortia at the

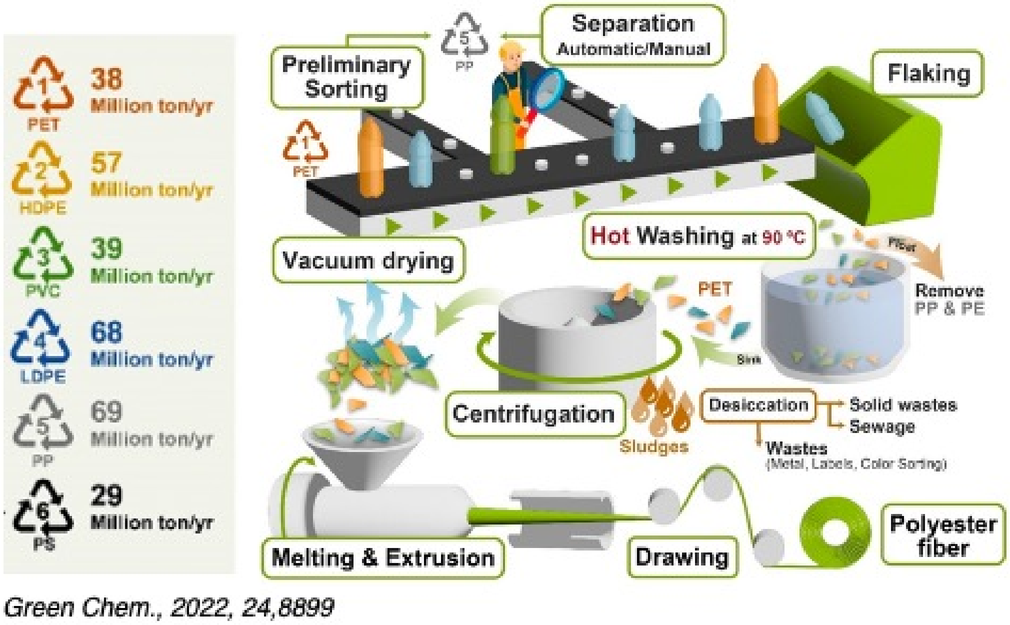


Figure 6-3: The six major commodity polymer chemistries and their approximate annual production (left) and the industrial process of mechanical recycling of poly(ethylene terephthalate) (PET) plastic film (right) [40].

National Renewable Energy Laboratories. These efforts have resulted in fundamental discoveries including the development of heterogeneous catalysts for the chemical recycling of polyolefins, pyrolysis technologies for converting polyolefins to smaller molecules that can be used as fuels, and bioremediation routes for the breakdown of PETs [15].

Recommendation 6.3: We recommend that NSF's efforts in translating recycling and upcycling chemistries focus on specific commodity polymers which are only sparsely recycled using current technologies: polyolefins (polyethylene, polypropylene), poly(vinyl chloride), and polystyrene.

Translation from the laboratory/benchtop to realization at > 100 Mt/year will require iterative discovery between lab-scale reactors, development level scale-up, and pilot-scale application. For example, the NSF-CCI has discovered several catalysts that decompose polyolefins, which make up a large fraction of consumer plastics including HDPE, LDPE, and polypropylene, but these polymers are only sparingly soluble in common solvents. As a result, these studies focused on reactions of the highly viscous polymer melt phase in the presence of a porous catalyst particles within small-scale reactors (gram scale), frequently with stir bars or paddle mixers. Scale-up to a larger volume batch-style reactor is not straightforward and will likely require designs utilizing polymer processing equipment such as twin screw extruders. While the field of chemical process engineering is focused on exactly the science of scaling from laboratory to manufacturing, plastics have historically presented unique problems due to their highly viscoelastic rheology and low thermal conductivity. The processing of monomers into plastic commodities inspired entire basic fields of research in polymer physics and rheology which may now be leveraged into translating upcycling reactions. Whie this will leverage existing research, significant translational activity will be necessary to understand processing routes that begin by handling a highly viscoelastic melt that is difficult to mix and tends to develop *hot spots* and potentially ends with a liquid or gaseous product. Moreover, this translational activity may inspire redesign of catalysts and supports that are tolerant to such treatment. Similarly, while both chemical and enzymatic catalysts have reached remarkable efficiencies, improving their tolerance to impurities typical in plastic waste streams is necessary requirement for scale-up [49].

Finding 6.4: While basic science discoveries are performed at small scale on pure materials, translational activity is needed to translate these discoveries to processing techniques appropriate for large-scale, highly viscous, poorly soluble, chemically impure commodity plastics.

Recommendation 6.4: Specifically regarding chemical recycling approaches, NSF-TIP should focus on development of processing routes amendable to commodity plastics degradation and catalysts compatible with large-scale processing of highly viscous plastics to advance new routes of chemical recycling towards translation. Similarly, the development of enzymes and catalysts that are tolerant to the impurities and additives in commodity polymers should also be supported.

6.2.2 Scale-up of biomass derived and biodegradable plastics

Biomass derived monomers allow for a pivot away from fossil fuel derived polymers and so potentially can decrease the carbon footprint of polymers. In addition, the biodegradablility of many biomass derived polymers is unquestionably of importance in situations where they are likely to leak through even a much improved recycling network into the environment, for example in ocean applications or near sensitive environments. Further, biodegradability is likely the best option in situations where polymers are used within composites with other materials from which they will be difficult to separate. Several plant-derived monomers and polymers have already been commercialized including poly(hydroxbutyrates) (Danimer Scientific) and polylactides (NatureWorks as well as several other suppliers).

New biopolymers that allow for increased efficiency in growth and conversion to plastics – for example by using lignocellulosic starting materials rather than sugars have recently emerged from the polymer science community. While some efforts focused on biomass derived plastics that were as similar as possible to existing commodity plastics, more recent significant advances have focused on efficient routes towards monomer and polymer production that inherently result in new polymer chemistries [59]. In this case, the processability and properties of the plastics and their durability are critical to enable translation to practice. Testing of this kind requires polymer synthesis on a scale (10s to 100s of grams) that is beyond that of a typical academic, basic science effort and falls within the purview of “development” scale-up as described earlier in this section.

Further, in most cases, academic work on new polymers is reliant on a single source of plant-based material and tolerance to both impurities and also species variations is unknown. Finally, understanding of synthetic and manufacturing routes to producing these materials at scale with properties comparable to current plastics are unknown. For example, while lignin-biomass derived feedstocks are much more abundant than the sugars on which prior biopolymers have been derived, they face challenges ranging from feedstock localization and transportation (form factor, water content, weight, location) to feedstock variability (species, environment, seasonality, process sensitivity). Scale-up in this case also requires iterative process design to understand sensitivity to these factors and to design plastics systems tolerant to the variability of feedstocks and minimize challenges of localization/transport.

Finding 6.5: In order to find market translation, biomass derived polymers must both have properties equal to or better than current plastics and have demonstrated inexpensive synthetic routes that are robust to variations in feedstock. Testing of processibility and durability requires a much larger scale of materials (>>kilogram) as well as equipment and safety practices unusual in academic settings.

Recommendation 6.5: Create development-scale synthesis capabilities to fully demonstrate the viability of biomass derived polymers as alternatives to current commodity materials. The equipment and practices for such a level of scale-up are not typically found in academic laboratory settings. We recommend NSF-TIP consider this as part of the facilities recommended in **R3**.

6.3 Sustainability, Economic Viability, and Life Cycle Analysis

Finally, and perhaps most importantly, the separation of plastic waste at the recycling plant is a major economic and time barrier towards the implementation of a recycling stream. While concepts regarding the efficient intensification of process designs that will eliminate this step have been proposed, see Figure 6-4 below, development of such catalysts will require iterative catalyst designs along with the corresponding process design. Similarly, the lifecycle analysis and scalability of biodegradable polymers are unclear due to the energy and transportation cost/efficiency of source production, the redirection of land toward plastics production instead of food production, and the fact that these materials inevitably decompose into carbon dioxide.

In each case, as breakthroughs are made with respect to reaction and processing efficiency, there are major impacts on the possible economic viability and potential environmental impact of the technology. Iterative life cycle analysis and technoeconomic analysis are critical aspects of informing the directions of development and scaleup as well as enabling critical, early decisions regarding viability. Several basic science efforts now incorporate high quality, detailed LCA[13]: these analyses make many assumptions about beyond lab-scale implementations in process design on which energy consumption and efficiency are highly dependent. In the area of sustainability, such analyses are critically important. Via our reading and the briefings organized by NSF for JASON, we identified several instances of “green washing” of plastic circularity proposals that appear on the surface to improve sustainability but which,upon further inspection, were found to be significantly energy consuming or waste producing .

---

[13] for example: `https://www.bottle.org`

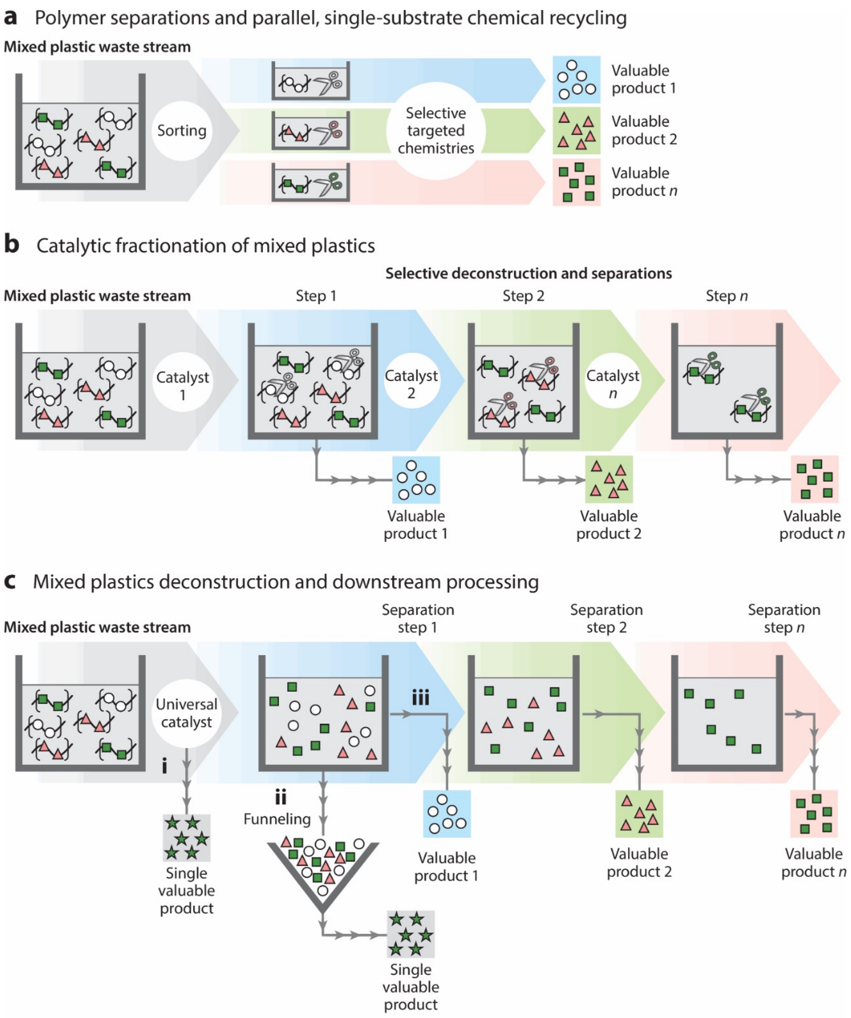


Figure 6-4: Plastic waste is inherently a mixture of many separate industrial plastics as well as additives. Process intensification strategies that either combine steps or result in the easier separation of small molecules (rather than plastics) are likely to dramatically improve the overall technoeconomics and lifecycle analysis of the endeavor. Here are shown some exemplary process frameworks for chemical recycling. (a) Plastic waste is separated followed by parallel, single-substrate chemical recycling. (b) A mixed plastic waste stream is sequentially exposed to selective catalysts which decompose specific components which are separated in turn. (c) A mixed plastic waste stream undergoes first a single-step reaction to a valuable product(i) or (ii) a single reaction to molecular intermediates, which would then undergo either a catalytic funneling process to a single valuable product or (iii) separation processes [49].

Finding 6.6: Life cycle analysis (LCA), encompassing materials, energy and water costs, environmental impacts, and technoeconomic analysis (TEA), encompassing a true comparison to the cost of existing technologies, are critical to a compelling value proposition. The LCA and TEA estimations improve as science and process design mature (**F7**).

Recommendation 6.6: Ensure that LCA and TEA are completed in-pace with iterative scale-up processes to give realistic feedback on the viability of plastic circularity solutions and to inspire problem solving (**R9**).

The organizations influencing the development of plastic waste solutions are many and complex, ranging from the plastics industry to recyclers to municipal waste representatives as well as the direct customers of plastics (e.g. consumer products companies). In this area, NSF-TIP's continuing relationship with these players is critical to shaping the details of any Requests for Proposals such that any output is relevant and actionable within this network. For example, we suggest that this is an ideal area for Consortia style funding that will allow for leverage of existing ”development scale” facilities within the polymer manufacturing industry, with the Consortia focusing primarily on the availability of data such that design rules and future AI/ML models can be appropriately trained. From our briefings and our own interactions with these companies, many have strong existing University Partnerships on which such interactions could be built.

6.4 Summary

While plastics waste is a pressing societal problem, translation of recent basic science breakthroughs requires:

- Scale-up to development scale synthesis and testing to fully understand system level integration challenges and materials properties;
- Concurrent and iterative life cycle analysis and technoeconomic analysis to drive process integration and demonstrate viability;
- This subject requires involvement in framing from the relevant industries to choose targets and to assure scalability of solutions into both manufacturing and waste streams.

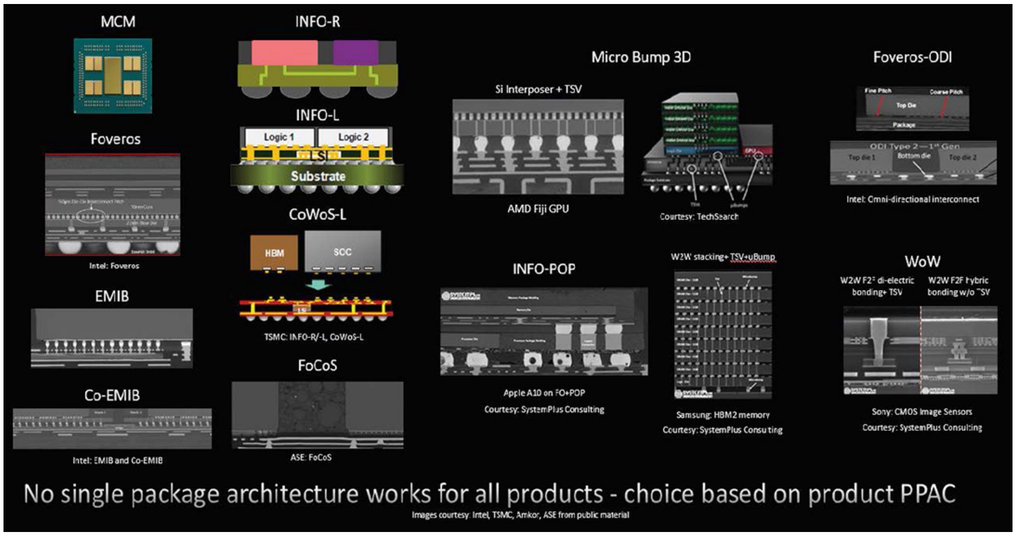
This Page Intentionally Left Blank

7 THERMAL AND PACKING CHALLENGES IN ELECTRONIC SYSTEMS

The explosion of high performance computing, connected electronic systems, advanced communications, IOT technologies, and mobile technologies have created an increasing demand for advanced electronics that permeate our everyday lives. For much of the past 50 years, our ability to increase the performance of microelectronics has followed Moore's law which postulated that the number of transistors on a chip would double every 18 months. Today, Moore's law is slowing as we are seeing the doubling of transistors every 2-3 years while the increase in high performance computing capability is doubling every 1.2 years. One major reason for this slowing is the increase of on-chip parallelism resulting in large heat fluxes and therefore a need for better heat management and packaging.

The role played by transistor miniaturization in advancing microelectronic circuit capabilities may be relatively easy to understand. Perhaps less well appreciated is the important role of "packaging" of those circuits. Packaging is done to place multiple integrated circuit (IC) chips onto a common substrate, protects the circuits against physical damage, ensures reliable electrical connectivity among all circuit components, minimizes signal loss and electromagnetic interference and *ensures effective thermal management.* For this reason, thermal challenges and packaging challenges for microelectronic systems must be considered concurrently. *As such, new materials that manage these challenges are a major "application-down" opportunity for NSF-TIP (Task 2) accelerated with the aid of AI/ML tools (Task 4).*

Today, advancements in modern high performance computing are being



No single package architecture works for all products - choice based on product PPAC

Images courtesy: Intel, TSMC, Amkor, ASE from public material

Figure 7-5: Imaging showing a variety of heterogeneously integrated microelectronics from major device manufacturers across the globe. The key aspect is the layout, bonding, and interconnection of chiplets and memory in a single package to create an advanced electronic system [63].

driven by innovations outside of the scaling of transistor density alone as predicted by Moore's law. The movement to each additional technology node in Si (e.g., 7 nm to 5 nm to 3 nm, etc.) is very expensive and time consuming considering the costs of processes like EUV (Extreme UV) Lithography, the development time necessary for manufacturing and improving yield, and the stress placed on advanced packaging. Thus, while the microelectronics industry continues to scale transistor density, the importance of technologies like heterogeneous integration [14] will become more and more important to the future advancement of electronic systems. The ability to manufacture such leading edge microelectronics is now a strategic national priority through the 2022 CHIPS and Science Act, which aims to increase the domestic manufacturing capacity in the U.S.

---

[14] Heterogeneous Integration refers to the integration of separately manufactured components into a higher level assembly that, in the aggregate, provides enhanced functionality and improved operating characteristics [31].

Another factor working against traditional 2D scaling is the fact that computing energy efficiency decreases with higher performance in CPUs that are scaled to smaller nodes [63]. Thus, the use of innovative 2.5D and 3D device architectures involving chiplets and heterogeneous integration (HI) technologies will be critical for the future of advanced computing while also addressing energy consumption. These advances are occurring just as the growth in large data centers, access to large data sources, and the revolution in AI/ML are demanding increased computational capability [38],[91]. This development brings additional demands related to microelectronic device design and manufacturing. At present, the architecture of heterogeneous integration for electronics is very complex and has taken on many different forms as illustrated in Figure 7-5.

Thus, the critical issues for new materials solutions for thermal management of Heterogeneously Integrated (HI) advanced microelectronics relate to:

- The higher thermal dissipation of advanced circuits.
- The close placement of circuits stacked on top of each other, or placed in close side-by-side proximity in a single package (a so-called System in Package, SiP).
- The multiplicity of different interfaces and diverse thermal pathways for these HIs.

Finding 7.1: Advances in modern high-performance electronics depend on more than scaling to smaller feature sizes and higher densities. Innovative 2.5D and 3D device architectures composed of multiple chips and chiplets, e.g., Heterogeneously Integrated (HI) Systems in a Package (SiP), will be critical for future advanced computing. These architectures will require new materials solutions for thermal management and packaging (**F10**).

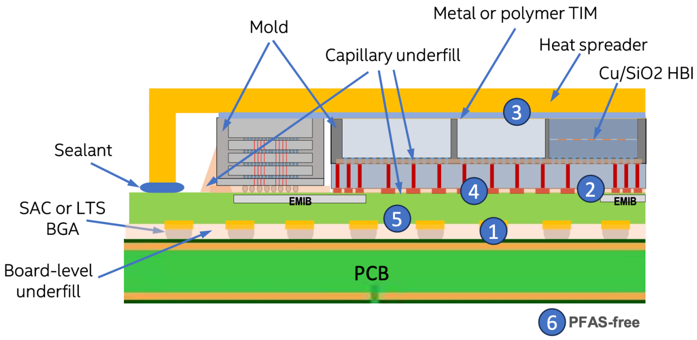
The remainder of this Chapter provides the background analyses of these challenges, as well as provides suggestions for meeting those challenges.

- Section 7.1 provides the broader context of needs and opportunities for new materials for packaging in general. The full set of materials needs is discussed since "thermal materials", such as "heat spreaders" will need to be compatible with all materials used in the package.
- Section 7.2 discusses the heat dissipation characteristics of current-day Si-based circuits used within microprocessors, as well heat dissipation of RF and high-power electronics. The discussion here again emphasizes the need for systems-level considerations.
- Section 7.3 discusses the systems-level complexities of modeling and simulation of such SiPs, important to address, even if only focusing on thermal issues alone.
- Section 7.4 discusses the importance of carrying out strategic experiments, and gathering data for the complex systems-level models, and advises on opportunities for AI/ML in developing those models.

7.1 Opportunities for Advanced Materials in Packaging and Thermal Management of Microelectronics

In his presentation to JASON, David Xu (Intel) described several key areas for materials innovation for future packaging and thermal management for microelectronics. This report will focus on issues of *thermal and interfacial challenges.* However, it is useful to have a broad overview of the application contexts beforehand, and thus we introduce this discussion here. The materials needs are schematically shown in Figure 7-6, and include:

Key Materials in an Advanced Package



1 New Interconnect Materials – lower temperature assembly
2 New Encapsulant Materials – polymer / polymer composites
3 Enhanced Thermal Solution – thermal materials for system
4 Interfacial Engineering – gradient interfaces & bulk layers
5 Power Delivery Materials – high-permiability low-loss magnetic materials for integrated voltage regulators
6 PFAS-free Materials – response to EPA PFAS regulations

David Xu, Intel

Figure 7-6: Key materials that will be required in advanced packages for future heterogeneously integrated IC.*D. Xu, briefing to JASON*

1. **New interconnect materials** for lower temperature hybrid bonding or assembly of heterogeneous devices onto a printed circuit board (PCB). Current temperature levels cause flexing in the components and printed circuit boards. This compromises the quality of the interconnects, and hence of circuit operation.

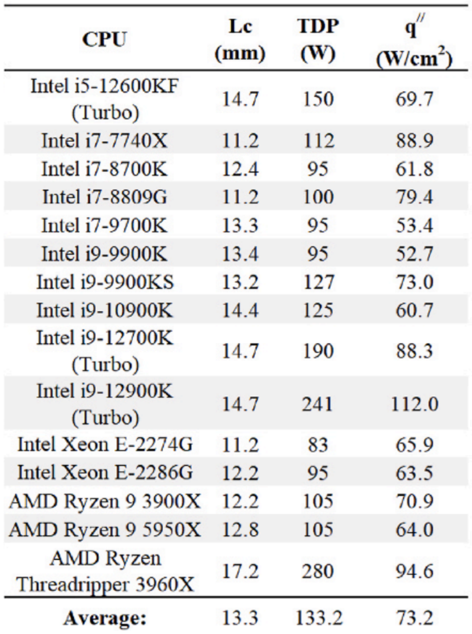
2. **New encapsulant materials** are largely formed of polymers or polymer composites. These materials must fully surround the space between the chips and their substrate, and also have appropriate values of adhesion, limited moisture absorption, and coefficients of thermal expansion (CTE).

3. **Materials for enhanced thermal solutions** assist in thermal management, such as those that may be used as *heat spreaders*, preventing the occurrence of "hot spots" in the circuits, and which are effective in removing heat from the SiP.
4. **Materials for interfacial engineering** provide better matches across interfaces, assuring that components continue to "stick together" with desired thermomechanical behavior and aid in the reduction of thermal interface resistance that results from phonon thermal transport processes. The incorporation of these materials enables low thermal stress, avoidance of sharp thermal gradients, and promotion of adhesion at interfaces and coating by encapsulants.
5. **Power delivery materials** that provide and control the electrical power to microprocessors and other high power components. Such materials might include high permeability, low-loss magnetic materials for integrated voltage regulators.
6. **Perfluoroalkyl substance (PFAS) material replacements** for the numerous PFAS-containing materials that span numerous applications. Further discussion on this issue is given in Section 8 in this report.

7.2 Present Challenges in Thermal Management for Microelectronics

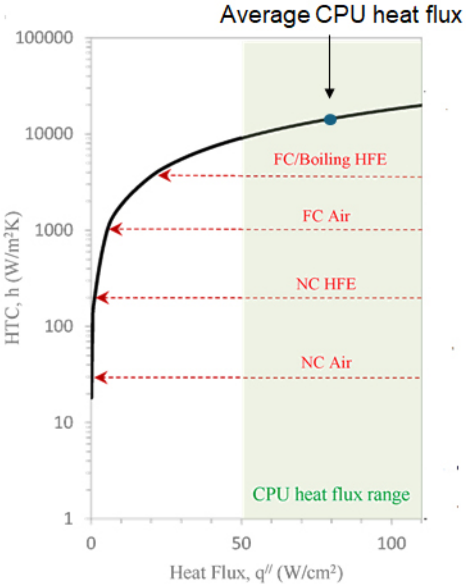
7.2.1 Thermal issues for HI SiPs

Appropriate thermal management of these heterogeneously integrated systems is necessary to ensure that devices do not exceed their temperature limits. Those limits are defined by device performance and reliability metrics. The ability to dissipate thermal energy and meet temperature limits is complicated by the increase in device heat flux within the complicated 2.5D and 3D architectures.



CPU	Lc (mm)	TDP (W)	q'' (W/cm^2)
Intel i5-12600KF (Turbo)	14.7	150	69.7
Intel i7-7740X	11.2	112	88.9
Intel i7-8700K	12.4	95	61.8
Intel i7-8809G	11.2	100	79.4
Intel i7-9700K	13.3	95	53.4
Intel i9-9900K	13.4	95	52.7
Intel i9-9900KS	13.2	127	73.0
Intel i9-10900K	14.4	125	60.7
Intel i9-12700K (Turbo)	14.7	190	88.3
Intel i9-12900K (Turbo)	14.7	241	112.0
Intel Xeon E-2274G	11.2	83	65.9
Intel Xeon E-2286G	12.2	95	63.5
AMD Ryzen 9 3900X	12.2	105	70.9
AMD Ryzen 9 5950X	12.8	105	64.0
AMD Ryzen Threadripper 3960X	17.2	280	94.6
Average:	13.3	133.2	73.2

(a)



(b)

Figure 7-7: (a) The increasing heat flux generated by modern CPUs. (b) The graph shows the convective heat transfer coefficient, h needed to remove a range of heat fluxes, q'', from a CPU with a characteristic length of 13.3 mm. The different means of convective heat removal include natural convection (NC) in air or a dielectric liquid (HFE), and forced convection (FC) in air or boiling dielectric. The *junction temperature* of the CPU is assumed to be at a maximum value of $T = 90°\text{C}$, with the coolant held at 35°C. [20]

For example, recent estimates of CPU (central processing unit) total power dissipation and heat fluxes show an average power dissipation of 133 W and an average heat flux of 73 W/cm^2 for chips with an average characteristic area of 177 mm^2. Figure 7-7 illustrates the challenges presented by these heat fluxes. The convective heat transfer coefficient required to remove 73 $\mathrm{W/cm^2}$ from the average CPU is greater than 10 $\mathrm{kW/m^2K}$ for a junction-to-ambient-temperature difference of 55 K. Such heat transfer coefficients can only be achieved by liquid cooling technologies, which are difficult to introduce at the chip level. Based on the IEEE Heterogenous Integration Roadmap [31], the average power and hotspot peak power densities for 2D and 3D device architectures are expected to exceed 200 $\mathrm{W/cm^2}$ and 900 $\mathrm{W/cm^2}$, respectively. Thus methods that can easily distribute or "spread" the thermal energy will be key for advancing the design and performance of HI microelectronic systems.

Moreover, while it may be desirable to place memory directly on top of the logic chip in a 2.5D or 3D package in order to shorten electrical access times, the high power dissipation and temperature rise from the logic chip would degrade the functioning of the memory elements. Thus, the placement of logic and compute chips within a *System in Package* (SiP) may require a trade-off between managing high heat fluxes and satisfying the designed performance metrics. Therefore, management and mitigation of thermal issues in HI electronics is a key area of future innovation that will enable their advancement.

7.2.2 Thermal issues for RF and high-power electronics

Modern wide bandgap semiconductor devices for RF and power electronics are the backbone of future high performance RF communications networks, advanced radar systems, and power electronics for the electrification of many industrial and transportation systems. While these devices may not be as highly integrated as the HIs described in Section 7.2.1, the average heat flux for such devices can exceed 1 $\mathrm{kW/cm^2}$. Thus, thermal management is a bottleneck that will limit the optimal performance achievable from these devices and the critical industrial applications they will be able to address. In a recent statement relevant to the DARPA THREADS program for advanced GaN RF electronics, DARPA Program Manager Tom Kazior noted that, “If we can relax the heat problem, we can crank up the amplifier and increase the range of radar.......by a factor of 2x to 3x [70].”

For wide bandgap devices, several figures of merit for RF and power electronics performance scale positively with the increase of bandgap of the semiconductor material [68]. However, in choosing materials with increasing bandgap from SiC to GaN to ultrawide bandgap materials like AlGaN and Ga_2O_3, there may be a *decrease* in thermal conductivity by an order of magnitude to values as low as 5 W/mK. Such a decrease would have an impact on thermal and packaging issues that range from the device to the circuit level. us, the development of some of these future electronic systems will require greater attention to materials integration to assist with heat dissipation in wide bandgap electronic systems. Recent development over the past three years have pointed to the fact that materials like doped AlN have some promise for creating electronics and would address both the need for wide bandgap and high thermal conductivity. However, these materials are in their nascent stage of development.

Heat spreading technologies can be effective in reducing the overall heat flux and temperature gradients in electronics while implementing active cooling schemes that efficiently dissipate the thermal energy. Researchers have demonstrated that the integration of diamond thermal spreaders in wide bandgap semiconductor devices has improved the performance of GaN RF transistors [42] (Figure 7-8). The growth of diamond layers onto wide bandgap semiconductors must be performed in a way that is compatible with the targeted semiconductor device behavior while also limiting the thermal stresses and warpage of the die or semiconductor wafer. Improvements in thermal resistance between the diamond and GaN layers have been achieved by introducing thin interfacial layers of

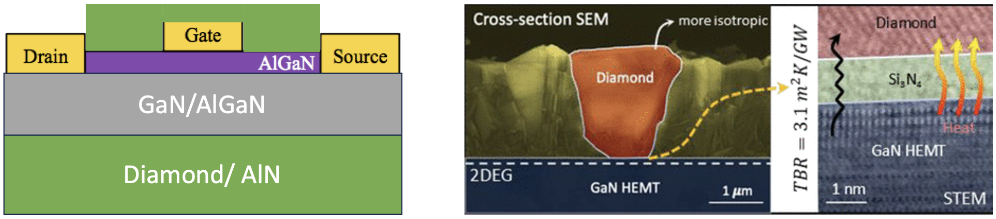


Figure 7-8: (Left) Image depicting the integration of high thermal conductivity heat spreaders with GaN or AlGaN high electron mobility transistors. (Right) The implementation of diamond on GaN transistors by researchers at Stanford University showing record low interfacial thermal resistance for the removal of heat from the device channel [42].

silicon nitride or silicon carbide that help to bridge the phonon density of states mismatch between the diamond and GaN, resulting in interfacial thermal resistances as low as 3 m^2K/GW. Thus, the efficacy of a *thermal management strategy* is dependent on well-considered *interfacial engineering* that matches materials properties across interfaces of devices and packages. Moreover, introducing heat spreaders at production scale poses additional challenges.

Finding 7.2: High power electronics generate large heat fluxes at the die level. Academic and small research laboratories have introduced materials with thermal conductivities above 300 W/mK as heat spreaders, including AlN, BAs, and diamond into such devices. Interfacial engineering has enabled the advancement of the integration and performance of these technologies. However, these are not all integrated through scalable manufacturing methods and limit the transition of this solution to high power/high heat flux electronics.

Recommendation 7.1: NSF TIP should fund the integration of high thermal conductivity heat spreaders at the die level into scalable fab-level manufacturing methods. This includes direct growth or deposition of these layers, bonding, and the tailoring of interfacial chemistry and properties to enable advanced heat spreading solutions at scale. Moreover, materials innovations and surface chemistry that can enhance heat removal through liquid cooling should also be considered.

7.2.3 Challenges imposed by interfaces: Thermal interface materials

As mentioned in Section 7.2.2, understanding of the interfaces between different materials is critical for the understanding of thermal management. Thus, when moving from the die to other levels of the device architecture, *thermal interface materials* (TIMs) are needed to reduce the thermal resistance in the heat flow path to the thermal sink used for cooling the device. Thermal interface materials can take the form of metals (e.g., solders), thermal greases, polymers, carbon nanomaterials, and other high thermal conductivity materials.

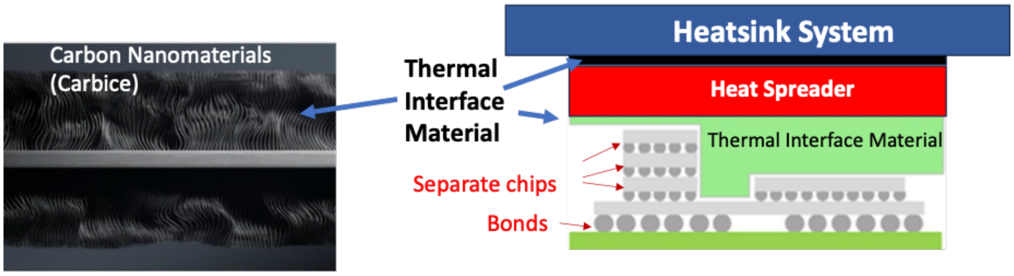


Figure 7-9: (Left) Image of carbon nanomaterial thermal interface materials from Carbice Corporation (image courtesy of Baratunde Cola). (Right) Depiction of thermal interface materials being used to join HI microelectronics to a heat spreader and the heat spreader to the heatsink system. Two different types of thermal interface materials requires are needed at each interface due to the topography and heterogeneity at the device level and the planarity at the heat spreader to heatsink level [4].

Challenges occur in the integration of such materials, and are particularly demanding at the manufacturing scale. These can include:

1. High processing temperatures. Due to the CTE mismatch and temperature limitations of some electronic components, the processing of thermal interface materials at elevated temperatures can introduce residual stresses, warpage, and other undesirable effects. Thus, reducing the processing temperature, especially for metal thermal interface materials, while maintaining excellent bonding and low thermal resistance is critical. Materials such as nanoparticles, sintered or transient liquid phase bonded systems may provide some solutions to this issue.

2. Mechanical compliance. When creating a thermal interface across two materials with different coefficients of thermal expansion (e.g., dielectrics/semiconductors and metals, etc.), residual stresses and cyclic thermomechanical loads are introduced that may result in reliability issues. Thus, developing low thermal resistance and mechanically compliant interfacial materials can be of importance to address this issue. The development of carbon nanomaterials such as those developed by Carbice Corporation from the DARPA nTIM program, have shown promising capabilities. Other forms of compliant and low thermal resistance thermal interface materials are still needed.

3. Accommodating structure and topology. In heterogenous integration, a topography may be formed due to the difference in heights of various chiplets and memory regions. Thus, thermal interface materials must be able to accommodate such topography during the reflow or attachment process (cf., Figure 7-9).

Finding 7.3: New materials are needed to reduce thermal interface resistance and thermomechanical stresses within packaged electronics.

Materials may include carbon nanomaterials, metal interconnects, and polymer composites.

Recommendation 7.2: NSF TIP should fund scaling and translation of thermal interface materials (TIM) informed by system requirements. These materials must bond at low temperature and can enable new topological designs.

7.2.4 Systems level considerations for thermal and packaging challenges

The discussions of thermal and interfacial management given in Sections 7.2.1, 7.2.2, and 7.2.3 reveal the importance of considering the appropriate *systems level solutions*. Optimal heat-spreading materials for power electronics may not be compatible with the materials and processing used for silicon-based HI SiPs. Moreover, these solutions cannot be implemented through a singular lens of thermal management since thermal effects are coupled to other critical device parameters as they can impart mechanical stresses, cause warping, and modify electrical properties. The effects are exacerbated when the electronic designs necessitate the use of heterogeneous materials with different coefficients of thermal expansion and different mechanical and electrical properties. Thermal expansion mismatch in assembling heterogeneous structures is a pervasive source of device failures from delamination and crack propagation to low yields during manufacturing to inefficient thermal management and device reliability. Furthermore, any solution has to be amenable to scalable manufacturing. The multi-materials, multi-physics, and engineering complexity of satisfying systems-level performance also informs the modeling and simulation requirements, as will be discussed in Section 7.3.

Finding 7.4: Advanced microelectronics systems (such as HI in SiPs) exacerbate challenges in thermal management, offering opportunities for new materials and material systems solutions. Thermal effects in such HI systems are strongly coupled to electrical and mechanical performance, and materials solutions for these “Thermal Interface Materials” (TIMs) must also accommodate these constraints(**F11**).

Recommendation 7.3: NSF-TIP should fund research projects that model, process and evaluated possible TIMs within a systems context. This will lay the foundation for a long-term better match between research innovation and industrial adoption in advanced materials for microelectronics (**R10**).

7.3 Modeling and Simulation for Materials Integration

The development of advanced computational tools to aid in the design, manufacture, and performance of advanced semiconductors is critical to improving their development cycle and to the translation of materials into systems-level applications. These computational tools can lessen the risk in adoption of new materials and device architectures needed to advance electronics capabilities and improve thermal management systems. Figure 7-10 schematically represents the challenges for modeling and simulation at the systems level. Modeling and simulation methods for these HI SiPs will have to span many orders of length and time scales to capture important details for robust design of the SiP. Currently, the details of electrical design and analysis are largely customized for each component; the different tools and methodologies used for the different components provide challenges in systems-level integration. The strongly-coupled nature of electrical, mechanical, and thermal interactions requires that package-level details, such as mechanical stress and warping, must be integrated into the modeling and design of the

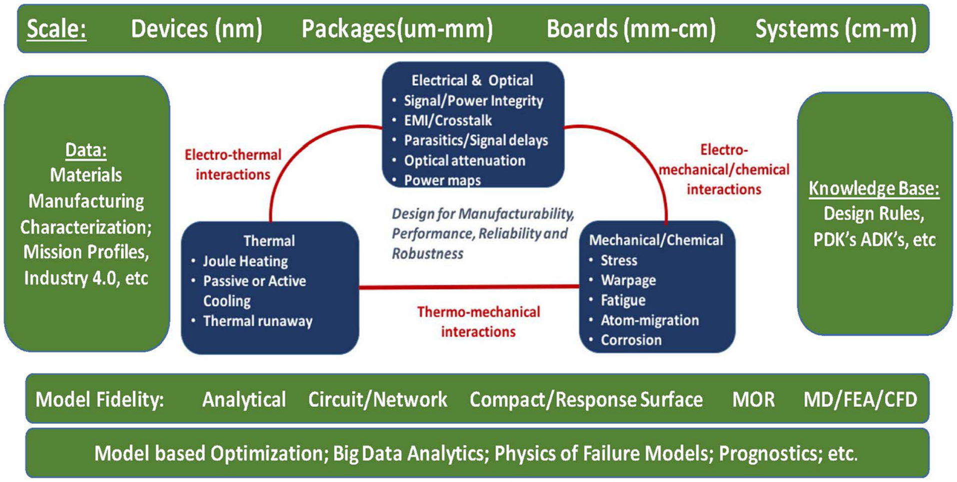


Figure 4: Modeling and simulation to inform the knowledge-base for heterogeneous integration

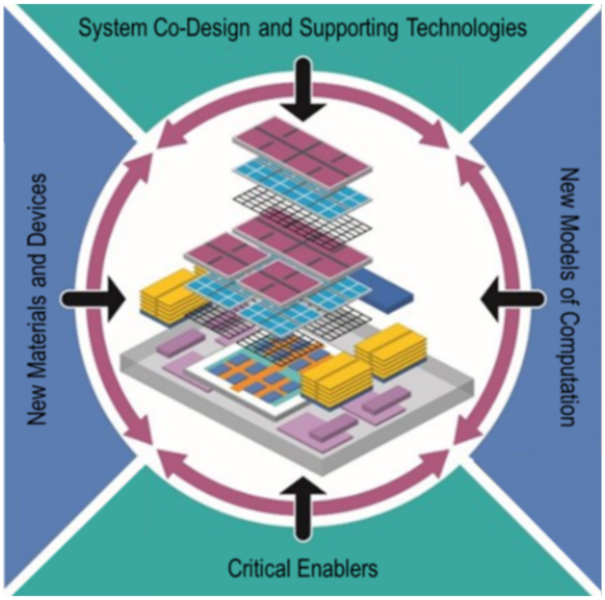
Figure 7-10: Modeling and simulation of advanced, heterogeneously integrated (HI) microelectronics systems in package (SiP). The broad range of dimensions (scale) that are encompassed and the coupling of electro-thermal, electro-mechanical, and thermo-mechanical interactions involved illustrate the complexity of demonstrating suitable materials solutions for these systems, as well as the challenges of modeling and simulation. Materials data (left-hand side) must eventually be translated into the *Process Design Kits (PDKs)* and *Assembly Design Kits (ADKs)* shown on the right-hand side, that provide the design rules for manufacturing [31].

system at the early stages. Accurate knowledge of materials parameters is critical for effective modeling, as are the details of the processes used to form the electrical and packaging components. Full-scale, systems-level modeling serves an important role in initial considerations of new materials into applications, but the range of informed, integrated models required appears daunting.

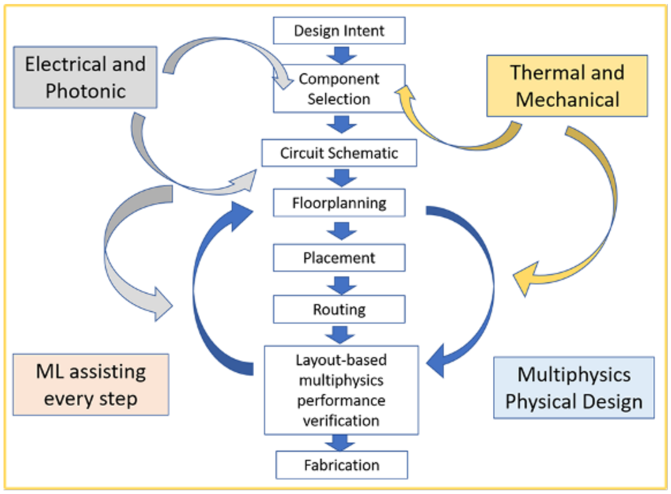
A solution that might augment improved physics-based computational tools is the addition of AI/ML approaches to further advance the computational toolset available to the semiconductor industry. Such tools can play a critical role in enabling the integration of new materials into devices while exploring their potential implications on manufacturing, device performance, and reliability. For example, a recent news release by Intel corporation noted the role of internally-developed Augmented Intelligence tools substantially reducing the analysis time (weeks to minutes) of sensor placement for measuring hot spots in chip designs. Such tools have already been used to design Intel mobile processors, like Meteor Lake [32].

AI data-driven methods can provide powerful augmentation of physics-based models. However, the development of these tools is uneven across the semiconductor industry and would benefit from NSF investments to ensure that the fundamental foundations are improved for both physics-based and AI-based models. Moreover, as is generally true for ML approaches, it is imperative that a large body of data be collected, appropriately catalogued and formatted, and curated in order for AL/MI techniques to be effective. Such data extend over individual materials and their structural, electrical, and thermo-mechanical properties, but must also include details of the processes used to assemble materials into the final microelectronic SiPs.

An example of a rapid design ecosystem that leverages AI/ML approachers is being developed for HI microelectronics at Purdue University and is shown in Figure 7-11 [55]. This framework provides a clear path for new materials and devices to be combined with co-design technologies, advances in computational models, and other critical enablers (e.g., computational hardware, etc.) to improve the design and adoption of new HI devices that incorporate advanced materials. The framework delineates a range of steps from design intent through fabrication where AI/ML along with multi-physics models are combined to help new architectures progress from concept to reality. This framework enables the properties of new materials and other critical



(a)



(b)

Figure 7-11: (a) Image depicting the computational ecosystem for HI microelectronics design which accounts for new materials and devices along with system-level co-design and new computational tools that will reduce the cycle time for designs while also de-risking the introduction of new materials. (b) Additional detail of the physics-based models integrated with AI/ML tools to improve the process of device design intent through fabrication. Images are from the Rapid HI Center at Purdue University [54].

parameters to be introduced through electrical, thermal, and mechanical models to provide a test bed for early predictions of the impact of materials on device behavior.

As more data are gathered for specific device architectures, the refinement of these modeling ecosystems from real world data will help to improve the viability of these approaches. It is important that the data include accurate materials, device and processing parameters, to fully inform ML and AI. Ways of collecting such data will be discussed in Section 7.4.

Finding 7.5: Modeling and simulation are crucial for directing materials choices and strategic testing for the thermal performance of high-performance integrated HI system. Modeling tools need to be extended to cover the full range of length scales and include thermal-electrical-mechanical effects across the numerous interfaces in these systems. Additionally, simulations must consider details of how HI systems are assembled, such as the methods of materials deposition (**F12**).

Finding 7.6: AI and ML can improve the quality of modeling and simulation of materials for thermal and interfacial management of microelecronic systems, but can only achieve this with an extensive, well-catalogued and curated database of necessary materials and process parameters, along with system-level performance data. Data collection should be explicitly structured to enable the investigation and quantification of process-structure-property relationships through AI/ML (**F13**).

Recommendation 7.4: NSF TIP, in partnership with other areas of NSF and other organizations funding basic research, should fund the development of multi-scale, multi-physics systems-level models for thermal management in HI systems, including coupled thermal-electrical-mechanical effects (**R11**) .

7.4 Informed Modeling and Simulation: Data Collection and Accelerated Development

As noted in Section 7.3, the complexity and diversity of length and time scales, as well as of component materials, requires the incorporation of a tremendous range of cross-cutting data. For a non-standard material, new processing and testing procedures need to be developed to create and analyze the demonstration device and the prototype, using existing, standard machines to develop a new technology. By contrast, manufacturing requires established procedures using dedicated machines for volume production using a manufacturing process that may have been locked in several years before production actually takes place. Section 6.1 discussed the process of translation from a materials design to industrial practice, delineating the importance of an iterative process where scale-up effort will inform new scientific challenges that must be addressed. For the microelectronics industry, the disparity in time scales between research innovation and industrial implementation is particularly acute, as indicated in Figure 7-12. The microelectronics industry does not generally take on the risk of accepting lab scale solutions without significant technology or market pull. *Development scale* demonstrations of materials applicability will play an important role in gaining acceptance of new materials solutions.

As discussed in Section 4, facilities that enable expansion beyond laboratory-scale experiments and models are essential for addressing scale-up challenges (**Finding F3**). Moreover, appropriately-focused pilot facilities offer the opportunities for well-controlled, automated device and package processing, and testing, also offering the opportunity for collecting and labeling process and test data that will better inform AI/ML approaches. To allow accelerated development of materials to address thermal and packaging challenges, such facilities could include:

1. Facilities for controlled and monitored integrated processing at the *development scale* (see Section 4.1), e.g., bonding, encapsulation.
2. Characterization and test facilities for multi-level, multi-property SiP testing for the research community.

As discussed in Section 4, these facilities would also serve the dual purpose of providing much-needed data on the processing details and characterization outcomes of materials within an applications context, offering opportunities for the collection, cataloguing and curation of data to inform the use of AI/ML approaches that could inform development scale demonstrations and shorten the time to industrial acceptance.

Finding 7.7: For the microelectronics industry, the mismatch with the research community in timescales for translation readiness and systems-level validation is particularly acute. Industrial process details and quality-control monitoring are generally not open to the public.

Recommendation 7.5: NSF TIP should leverage and expand existing facilities to pilot multi-level, multi-property SiP testing for the research community, establishing well-calibrated procedures for such testing (**R12**).

Recommendation 7.6: NSF TIP should partner with other relevant government agencies to create pilot facilities for simple, but well controlled and monitored, integrated processing for HI microelectronics thermal management. These pilot facilities should collect and curate processing-related and systems-level performance data, which will enable AI/ML -facilitated system-level thermal, electrical, and mechanical models supportive of new materials integration (**R13**).

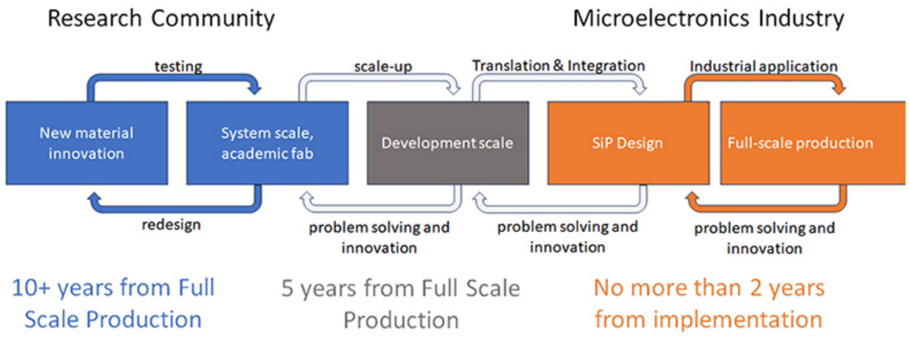


Figure 7-12: The process of translation from a materials design to industrial practice for the microelectronics industry demonstrates a distinctive mismatch of time scales. Post-lab-scale demonstrations are critical if materials innovations are to cross the Valley of Death from innovative material to systems-level enabler.

This Page Intentionally Left Blank

8 ALTERNATIVES TO FLUORINATED COMPOUNDS IN MATERIALS FOR NATIONAL AND ECONOMIC SECURITY APPLICATIONS

8.1 Ubiquity of PFAS in Applications with Unique Requirements

Fluorinated materials have penetrated nearly every aspect of modern life. Teflon™, the most recognizable fluoropolymer, is highly anti-fouling and used ubiquitously not only in non-stick and anti-stain household items, but critically in biomedical applications including stents. Other fluoropolymers are used as everything from lubricants to high temperature tolerant o-rings and electrochemically stable membranes. Fluorinated small molecules are not only common refrigerants, but also critical to semiconductor manufacture as a highly light absorbing compound in photoresists, barrier coatings, and anti-reflective coatings. From a consumer perspective, PFAS's appear in a ubiquitous number of products, as shown in 8-13 below.

In April 2024, the US Environmental Protection Agency mandated that water providers reduce the perfluoroalkyl and polyfluoroalkyl substance contamination in drinking water to 4 parts per trillion [74]. Nearly simultaneously, 3M agreed to pay $10.3B to assist in public water suppliers in PFAS removal efforts [2] and also announced their abrupt exit from the production of all perfluorinated alkyl substances by 2025 [3].

The exit from the market of the world's leading manufacturer of a number of compounds that are ubiquitous in modern life is already having ripple effects throughout the economy. One major concern is that

Figure 8-13: Perfluoroalkyl substances (PFAS) are incorporated not only in fluorinated plastics like Teflon™, but in a vast array of consumer products. Concerns regarding health combined with the abrupt end of manufacture of many key reagents are likely to dramatically upset supply lines in the near future. The development of new materials and formulations with similar stability and surface properties is urgently needed [17].

these materials are very difficult to replace in critical applications due to their toughness combined with high heat and chemical stability as well as low friction qualities. For example, Teflon™is the prevalent material used in both biomedical stents as well as tubing used in semiconductor manufacture. Similarly, the carbon-fluorine bond makes Nafion™uniquely stable for electrochemical applications including electrolyzers and fuel cells. Finally PFAS are used in numerous national security applications including energetics, batteries, and microelectronics [1]. While toxicology studies continue and are currently unclear with respect to fluoropolymers such as Teflon™, one major concern regards whether they leach PFAS during production, use or upon disposal. While fluoropolymers do not appear to decompose easily, small molecule PFAS are routinely used in the manufacture of many fluoropolymers as a surfactant to enable aqueous suspension synthesis (among many patents in this space we reference the following examples of early patents in this area [10, 43, 9]). It appears that leaching of this small molecule is the primary source of leachable PFAS during manufacture and perhaps during use [69].

While it is likely that other countries will step in to to produce PFAS despite the potential environmental consequences, there will be increased competition for this now more-scarce material, and U.S. concern about PFAS leaking into the environment will also apply to any applications in which PFAS is used. Finally, in the national security applications, a domestic source of a replacement material is critical. This change in regulatory environment and availability of common reagents highlights a new and pressing need for translation of a number of technologies that were previously considered either too expensive or inferior in terms of properties when compared to fluorinated alternatives. *As such, development of alternative materials or processing methods suitable for applications of national and economic security concerns constitute a* *timely investment for NSF-TIP (Task 2) with significant opportunity to leverage newly developed AI/ML tools (Task 4).*

8.2 PFAS as a Newly Critical Material

A "critical material" was initially defined in the Energy Act of 2020 as: "Any non-fuel mineral, element, substance, or material that the Secretary of Energy determines: (i) has a high risk of supply chain disruption; and (ii) serves an essential function in one or more energy technologies [81]." While this definition was pointed explicitly at energy security, it is useful in thinking about the "criticality" of various PFAS products and applications. Specifically, criticality can be thought of through a plot of Importance to National or Economic Security versus Risk to Supply, as shown in Figure 8-14. Criticality is then defined as the set of applications and materials for whom the importance is high and there is also significant risk to supply due to availability.

Finding 8.1: The essential use concept [75] as well as the American Innovation and Manufacturing Act (AIM) protect or allow for continued use of essential products if use of a replacement substance is impossible or impractical. While these provisions address regulatory changes and allow for continued use, they cannot protect even essential uses from market constrictions that result in a loss of availability of products (**F16**).

The uses of PFAS have been under development for more than half a century, and products and processes have been developed based on the availability of PFAS, while PFAS-based materials have been optimized for product needs. Changing all aspects of supply chain; environment, health and safety (EHS) impacts; materials production; and incorporation in products in such a short time is a daunting challenge. Ideally, the essential use concept combined with the AIM act will allow a gradual

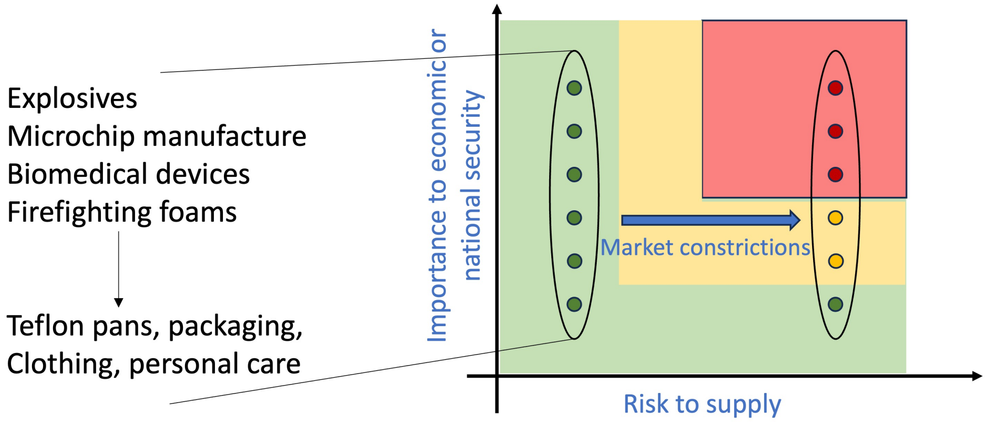
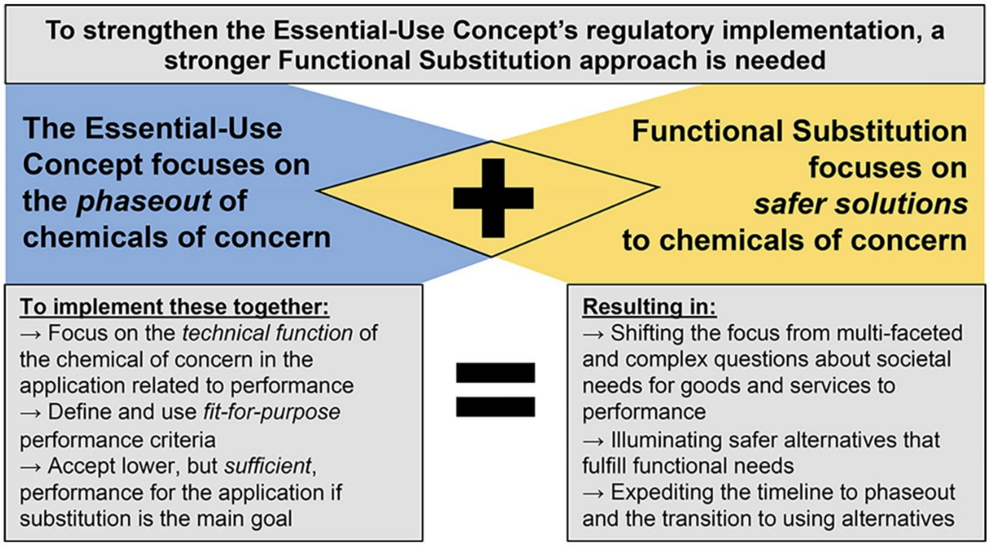


Figure 8-14: Critical Materials are materials with significant importance to national or economic security and also a high risk to supply. PFAS containing products are of varying importance, but due to increased regulations and market constrictions, these materials have moved significantly to the right on this plot in recent years, with some applications becoming critical. Figure adapted from [72]

.

phase out of PFAS as replacements are created as illustrated in Figure 8-15. Unfortunately, it is not yet clear whether a new domestic manufacturer will appear to supply these materials, mitigating the market constrictions and supply risks. Regardless, the eventual phase out of even essential use applications motivates the rapid translation of alternative materials.

Market forces will drive the translation of many PFAS alternatives for the the consumer products illustrated in Figure 8-13 [75, 7, 51, 26, 39, 22]. However, highly demanding applications, particularly in those relevant to national and economic security, have stricter requirements that make replacements more difficult, including the need for requalification for new versions of an old product. The essential use concept and negotiations with 3M for remaining "on the shelf" supplies are likely to provide temporary solutions for these sectors, but translation of replacement



To strengthen the Essential-Use Concept's regulatory implementation, a stronger Functional Substitution approach is needed

The Essential-Use Concept focuses on the *phaseout* of chemicals of concern

Functional Substitution focuses on *safer solutions* to chemicals of concern

To implement these together:
→ Focus on the *technical function* of the chemical of concern in the application related to performance
→ Define and use *fit-for-purpose* performance criteria
→ Accept lower, but *sufficient*, performance for the application if substitution is the main goal

Resulting in:
→ Shifting the focus from multi-faceted and complex questions about societal needs for goods and services to performance
→ Illuminating safer alternatives that fulfill functional needs
→ Expediting the timeline to phaseout and the transition to using alternatives

Figure 8-15: In an ideal scenario, phase out of PFAS under the essential use concept will be gradual and balanced with the development of alternative materials or processes based on functional requirements that are matched to achieve performance requirements sufficient for the application, and within EHS constraints.

materials must occur in parallel. In the following we will illustrate this concept with examples for the microelectronic and semiconductor industry and for specific, demanding DoD applications.

Finding 8.2: PFAS supplies are likely to become constrained by market contractions and reduced domestic production. Market forces are already driving replacements for consumer products. The essential use concept and access to remaining supply lines will protect the immediate needs of the economic security and national security relevant applications, but the supply is now at risk, making these PFAS products *critical materials* (**F14**).

Recommendation 8.1: NSF-TIP should focus efforts on PFAS replacements that are critical to economic security, e.g., fluorine-free photo-acid generators for lithography in the microelectronics industry, and national security, e.g., DoD-specific applications, with particular attention to drop-in alternative materials to minimize disruption in essential uses (**R14**).

8.3 Materials Replacements and Modified Processing

The Department of Defense has compiled an extensive list of PFAS-based products in their inventory, and assessed which of those are presently impossible or impractical to replace with alternatives [1]. Several categories of materials and applications on the DoD list (e.g. textiles, fire-fighting foams, cleaning fluids, low demand application o-rings and seals) are in common with much larger consumer bases for which market forces are and will continue to drive alternative materials to market. These products might meet many mundane DoD needs, but certainly would not meet the standards for the most demanding DoD applications such as operating in harsh environments. In these cases, the materials involved may provide a starting point for a structured program of materials development to meet essential needs with more challenging standards, as will be discussed below.

8.3.1 Microelectronics and semiconductors

In one area that impacts both national and economic security, microelectronics & semiconductors, DoD reports that eliminating PFAS is impossible or impractical for essential uses, an assessment that is also expressed by the semiconductor industry [50, 58] as is shown in Figures 8-16 and 8-17.

The changes indicated in Figures 8-16 and 8-17 require significant R&D

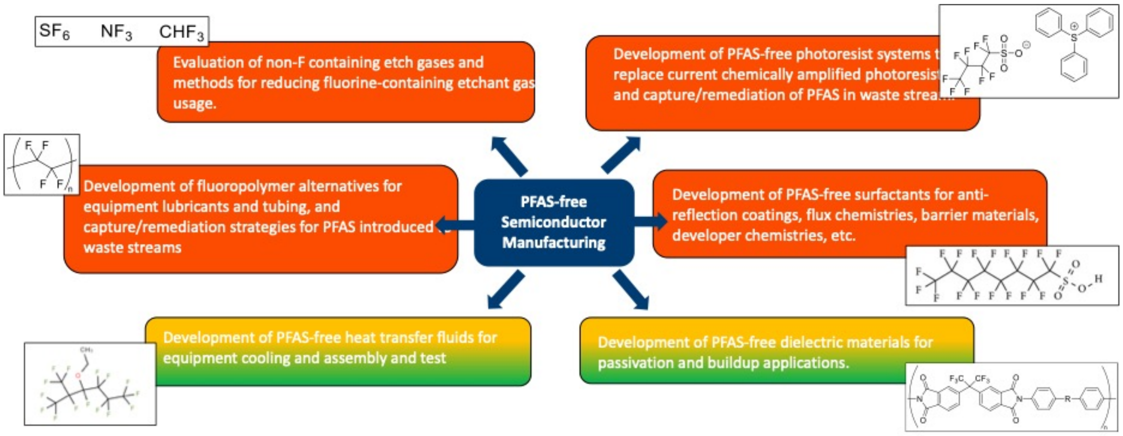
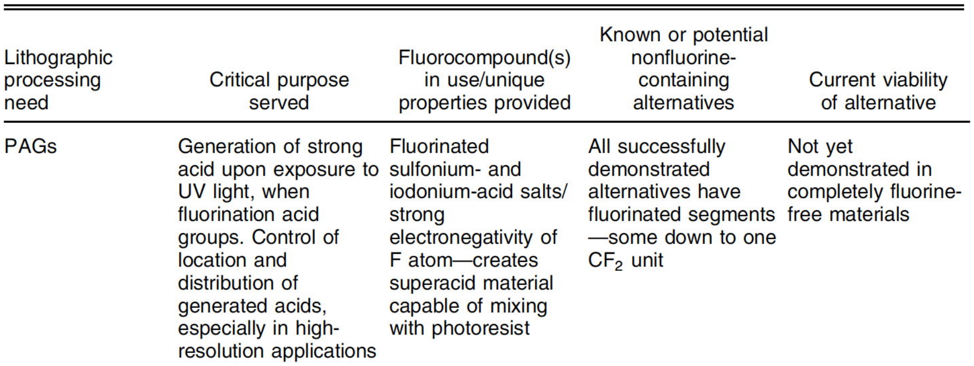


Figure 8-16: The semiconductor industry's use of PFAS ranges from the light absorbers (photo acid generators (PAGs) that allow for patterning of transistors to the tubing used in equipment. Intel's analysis color codes applications for which they have no readily available alternatives as red and areas where alternatives may be available as yellow. *Figure reproduced with permission from D.Xu (Intel), presentation to JASON*



Lithographic processing need	Critical purpose served	Fluorocompound(s) in use/unique properties provided	Known or potential nonfluorine-containing alternatives	Current viability of alternative
PAGs	Generation of strong acid upon exposure to UV light, when fluorination acid groups. Control of location and distribution of generated acids, especially in high-resolution applications	Fluorinated sulfonium- and iodonium-acid salts/ strong electronegativity of F atom—creates superacid material capable of mixing with photoresist	All successfully demonstrated alternatives have fluorinated segments—some down to one CF_2 unit	Not yet demonstrated in completely fluorine-free materials

Figure 8-17: Example of Semiconductor industry perspective of PFAS ban impacts on an individual lithographic step. PAGs are Photo Acid Generators, which are used to transfer patterns in photolithography. From Reference [50]

to identify new materials or processes, much of which is underway but has not yet been translated to industrial practice. Indeed, the Semiconductor Industry rule of thumb is that significant changes in materials and process will require a decade for implementation, as discussed previously in Section 7. In this case, it is likely that in many cases, the use of fluorinated materials in these markets will be deemed ”essential use” for the short term while R&D is required for future replacements. For the photolithography process, for example, there is a strong motivation to have a drop-in alternative to the fluorine-containing molecules now used for the photo-acid generator (PAG) materials [50, 37]. There has been research in this area that indicates viable molecular alternatives which could form the basis of a TIP funded translational and acceleration activity. Critical to this effort will be continuous evaluation of new materials and processes for environmental, health and safety (EHS) issues so as not to simply move from one environmentally restricted material to another.

Finding 8.3: Integrated dependencies of products and PFAS materials for both the microelectronics industry and for specialized national security applications have evolved over decades of co-development. PFAS materials are now critical to economic and security applications and are in some cases essential to performance of the relevant products.

For polytetrafluoroethylene (PTFE), there is no proven drop-in replacement material, and there is strong industry preference to modify the production process while maintaining the final material [6, 14]. PFAS-based surfactants are used in the polymerization to create PTFE and are the dominant source of water contamination related to PTFE. Alternative surfactants have been proposed [6, 14] and are being used in some markets [69]. However, there are concerns that the use of non-PFAS surfactants reduces control and uniformity in creating the end product [69]. Alternative solvents which eliminate need for surfactants, such as supercritical carbon dioxide have also been suggested in the past, but have not been developed up to full plant scale [19].

These examples are not atypical in developing alternatives to fluoropolymers. Often there has been prior research indicating possible alternatives, but these have not been pursued because there was little economic motivation to replace the dominant PFAS materials or process, or because the end product was not identical to the results from the original process. In the cases of PTFE and Viton (see below), with the threat of losing a valued market, fluoropolymer manufacturers are now aggressively pursuing changes in chemistry and process. The direct application of these new materials to the specific critical materials concerns (national and economic security) is an opportunity for TIP in terms of both advancing the translation of some of the above listed alternatives (which were only demonstrated in academic settings and also in formulating entirely new material alternatives). Specifically, the questions revolve around functionality and durablity (which lead to qualification) of the new alternative materials and processes under the specific, and demanding use conditions of these markets. While eliminating the surfactant is critical to producing fluoropolymers that are less likely to leach fluorinated compounds during use, parallel studies on the end-of-life chemistry of these materials are also necessary to ensure proper disposal.

Finding 8.4: In the prior decades of research and development, a vast amount of data, much of it proprietary to industry, has been amassed on the properties and synthesis of PFAS materials, as well as alternative materials that have been considered for similar functions. While much of this may be soon leveraged for near-term solutions, in some application cases, the Carbon-Fluorine bond in PFAS may be irreplaceable because, for example, it imparts extraordinary temperature and chemical stability. (**F15**).

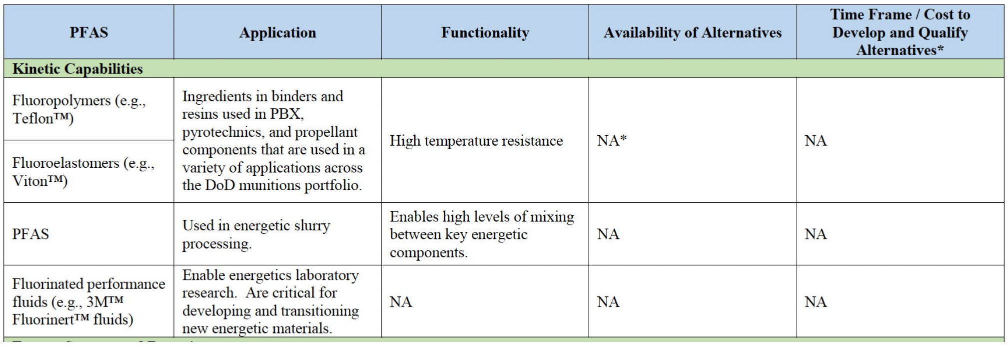
Finding 8.5: Several methods for alternatives to fluoropolymers or for alternative fluoropolymer manufacturing are being developed to reduce environmental leaching. Transitions to these alternatives will likely focus on large markets with less demanding requirements. Consequently, the DoD may struggle to find manufacturers for specialty versions needed for their essential use applications including binders for explosives and o-rings for demanding environments (**F17**).

Recommendation 8.2: For irreplaceable fluorinated materials in essential applications, NSF-TIP should prioritize translation of manufacturing and processing methods, with highest priority on eliminating environmental release, e.g., synthesis and manufacture of fluoropolymers that do not contain leachable fluorinated small molecule surfactants. (**R15**).

8.3.2 Unique DoD requirements – kinetic materials

Some DoD requirements have limited parallels in the private sector and very strict performance criteria. One example is kinetic (i.e., explosive) materials, illustrated in the DoD PFAS assessment shown in Figure 8-18. Binders for these materials have been fluoropolymers (*e.g.,*PTFE and FKM polymers (co-polymers of vinylidene-fluoride with other fluorinated monomers). The polymerization process for both polymers has traditionally used fluorochemical surfactants, discussed above for PTFE. Several chemical manufacturers have developed replacements for fluorinated surfactant resulting in a family polymers which do not require the PFAS compounds now under stricter regulation during manufacture and do not appear to degrade to or leach PFAS compounds, which has proven easier for FKM polymer products than for PTFE. However, changes in product performance must still be evaluated for both materials [69, 24] for meeting qualification criteria.

Finding 8.6: As a part of the National Science Foundation, NSF-TIP has access to a broad basic research platform and is therefore ideally



PFAS	Application	Functionality	Availability of Alternatives	Time Frame / Cost to Develop and Qualify Alternatives*
Kinetic Capabilities				
Fluoropolymers (e.g., Teflon™)	Ingredients in binders and resins used in PBX, pyrotechnics, and propellant components that are used in a variety of applications across the DoD munitions portfolio.	High temperature resistance	NA*	NA
Fluoroelastomers (e.g., Viton™)				
PFAS	Used in energetic slurry processing.	Enables high levels of mixing between key energetic components.	NA	NA
Fluorinated performance fluids (e.g., 3M™ Fluorinert™ fluids)	Enable energetics laboratory research. Are critical for developing and transitioning new energetic materials.	NA	NA	NA

Figure 8-18: Polymer-bonded explosives (PBX) contain fluoro-polymers (top two rows) and other PFAS-based chemicals. Other fluorochemicals are used to enhance mixing, and ‘Fluorinert‘ is used as a coolant in High Explosives development and test labs.

situated to accelerate the materials discovery and translation of PFAS alternatives needed by other agencies and missions.

Recommendation 8.3: NSF TIP should focus on translation of PFAS alternatives for application integration under use conditions (DoD, DOE-NNSA, and microelectronics) via systematic discovery, production and testing.

8.4 Data and Accelerated Development

In carrying out the transition away from PFAS, the data amassed in decades of industrial development will be invaluable in developing functional replacements to the extent that industrial collaborations support access to these data. The combination of essential use priorities and functional replacements for existing products, with a strong emphasis on EHS, as outlined in Figure 8-15 should shape the R&D timeline. The effective use of historic data, its augmentation and curation, may jump-start the effective use of AI approaches in reduction of time to deployment of PFAS alternatives. There is a natural complementarity here with the initiative on AI Aspiration for Sustainable Materials (aiA) [5].

Finding 8.7: The already-existing vast amount of industrial data on the properties and synthesis of PFAS materials and alternative materials can constitute a substantial and highly-leveraged data base for AI approaches that may be able to reduce time-to-translation of PFAS alternatives (**F18**).

Recommendation 8.4: NSF TIP should support the transition from PFAS by collaborating with industry on historic data and by implementing expanded Materials Genome R&D concepts under the AI Aspiration for Sustainable Materials [4]. This work will include supporting data bases of historical and new structural [12], physical and functional properties, as well as training data for processing procedures, all of which can then be used in accelerating discovery of candidate materials and processes (**R16**).

An important point of connection will be NSF's Convergence Accelerator project, PFACTS [77]. The PFACTS project is beginning by creating a database of commercially-relevant PFAS materials and their regulatory definitions. It will expand to include the industrial application requirements, the relevant physical properties of the materials, and potential alternatives. The goal will be to support computational [37] and AI materials discovery and optimization. NSF TIP can expand the impact of this project by supporting parallel data bases for potential promising alternative materials classes, and by supporting experimental programs to expand data bases to address synthesis and processing approaches.

It is certainly the case that existing data sources will not be found to hold all the information needed to realize the goals of the AI Aspiration for Sustainable Materials. NSF TIP can play an important role by supporting work to accurately identify the essential physical properties and their values (including experimental means where data are lacking) that are most important to design and synthesis of new non-PFAS-based materials. NSF TIP can also support experimental development of data about the evolution of materials along selected processing pathways, and the relationship to the properties of the final product. This will provide invaluable training data for computational chemistry discovery and AI optimization of production pathways for the desired new materials.

9 VIGNETTES ON OTHER CLASSES OF MATERIALS

The following subsections include materials that we believe may be rapidly approaching the “goldilocks” zone for materials translations. We include them for illustrative purposes along with signposts of advancements we believe will be signals of readiness for translation.

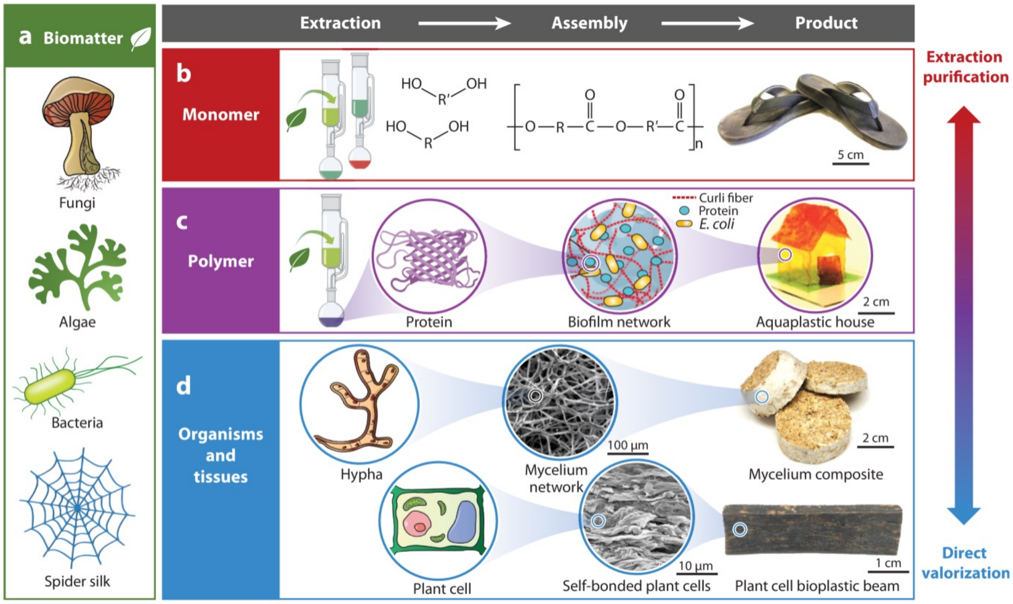
9.1 Bio-plastic Composite Materials

The area of Biomaterials research has the potential to integrate biological building blocks to form new materials with useful properties. The bulk of this research to date has focused on the development of materials that interact with the body, *e.g.,* tissue engineering, drug delivery, and other biomedical applications. In our study, however, we recognize a growing body of literature where similar strategies are being used to deliver new classes of bio-derived materials for applications ranging from sustainability (materials whose synthesis, manufacture, and disposal have lower life cycle impact on the environment) to self-healing. As illustrated in Figure 9-19, the integration of bio-derived substances into materials can take three general routes:

(i) The extraction of monomers from biological products to make polymers that may or may not be biodegradable (aspects of this work were covered in Section 6).

(ii) The extraction of full natural polymers and fibers, ranging from proteins and sugars to excretants such as silk and rubber, from biological sources that are then made into products.

(iii) The incorporation of full organisms or tissues into scaffolds to make new materials with hybrid properties that are, in effect, composites.



Campbell IR, et al. 2023
Annu. Rev. Mater. Res. 53:81–104

Figure 9-19: Paths to sustainable materials from renewable sources. (a) Sources of the biomaterials. (b) Polymers obtained via extraction of monomers, then synthesis. (c) Biopolymer extraction to create composite materials. (d) Polymer composites from building blocks of biological organisms. Waste and extraction needs increase from bottom to top. [13]

.

Here we are particularly interested in the latter category in which traditional polymers, chemically or biomass derived, are integrated with bacteria or other living materials into an integrated composite material [57, 13]. The idea is closely related to a traditional composite in which two separate components are co-engineered to yield a single material achieving properties of both constituents. During the JASON briefings we heard about the impacts of polymer/ceramic composites in making high strength, high tolerance coatings and other materials. This new version of a biological-polymer composite also seeks to achieve a material with new, enhanced properties over the traditional plastic, but in this case incorporating functions such as degradability or self-healing. For example, the presence of bacteria makes possible degradation of the polymer even in environments that lack microbes.

The great majority of the work on living biocomposites has been focused on biomedical applications, yet we find significant recent work on biocomposites aimed at creating a new class of materials made from renewable feedstocks with interesting properties. Below, we will briefly describe some recent advances in this area that show clear potential but conclude that there has not yet been sufficient fundamental investment to “push” forward translations. We recommend not only watching this area for signposts of translational readiness (similar to our conclusions on 2-D materials) but, in this case, also working with partners in the Basic Science focused parts of the NSF and other agencies to create more momentum as there is credible “pull” both in terms of societal excitement regarding sustainable materials and in terms of entrepreneurial efforts in these areas.

9.1.1 Sustainable Living Materials

There is a growing field of “engineered living materials” that aims to achieve beneficial properties owing to the inclusion of biological cells. For example, two recent research examples use 3D printing methods to embed biological cells in the printed material to achieve functionalities such as localized drug delivery [56] and patches for wound healing [27]. These methods are developing rapidly owing to the ready availability of additive manufacturing methods. In a non-biomedical application example, bacterial biomineralization has been harnessed to make self-healing concretes where the bacterial metabolic processes alter the pH and carbonate concentration of the matrix causing microbially induced calcium carbonate precipitation to occur and fill in cracks [18].

In the area of plastics, there are recent advances towards making new composites where bacteria, viruses, or algae are added during the plastic production process in order to contribute new functionalities including self-healing and reduction of the carbon footprint. There are several challenges, including

(i) using microbes that are not harmful in the environment;

(ii) identifying or adapting microbes to live and function during and after the high temperatures typical of polymer processing (e.g., $130 - 150$ °C);

(iii) the composite material should be as least as good as the original material;

(iv) for a process such as chemical degradation by a bacterium, it is necessary to understand the chemicals produced, since they may be different from other decomposition products of the polymer.

(v) because the microbes will be released in new environments, assessment is needed for the kind of competitive ecological changes produced by interactions with other native flora and fauna.

For example, in a recent paper, a polyurethane was prepared with the bacterium *Bacillus subtilis* to achieve a polymer with improved material properties (here, tensile strength) and which also was degradable, even when the plastic was deposited in an environment lacking microbes [34]. Note that polyurethanes (PU) are the sixth most produced plastic in the world and even though PU waste can be potentially collected under category seven of the corresponding resin identification code (see Figure 6-3, only 0.3 % of plastics in this category are generally recycled in the United States. Kim et al. [34] began with the observation that *B. subtilis* strains are known to have degradation activity against polyester-based polymers, and some *B. subtilis* strains can survive short times, *e.g.,* a few minutes, at temperatures as high as 100 °C, which, however, is still well below typical polymer processing temperatures.

The authors used the approach of adaptive laboratory evolution to demonstrate that they could enhance the heat-shock tolerance of *B. subtilis* spores. Moreover, in a step that is valuable for thinking long term about these kinds of approaches, they were able to identify the genetic basis for the measured enhanced heat-shock tolerance. They were then able to produce a composite of the evolved *B. subtilis* strain with polyester-based thermoplastic polyurethanes (TPUs), using a standard hot melt extrusion process. The bacteria survived both the thermal environment and shear stresses of the polymer processing; spores showed nearly full survivability (96â€“100 %). The authors then studied the mechanical properties, measuring an enhancement of toughness $\approx 25-37$ % compared to TPUs without spores. This result was interpreted similarly to other composite materials where the spores behaved as reinforcing fillers in the TPU matrix. Finally, as illustrated in Figure 9-20, the authors showed their biocomposite of bacteria and polyurethane (BC TPU), when placed in different landfill-like conditions, achieved over 90 % biodegradation at 37 °C in 5 months; the spores embedded in the TPU matrix triggered and facilitated the polyurethane biodegradation [34].

9.1.2 Biocomposite readiness for translational opportunities

While there are exciting prospect for living materials and a growing number of papers in this field, we identify it as one with insufficient "push" from fundamental discovery to fuel materials translation at the current time. It is our impression that the vast majority of fundamental work in this area has focused on health-related applications such as tissue scaffolding, the creation of biosensors, and schemes for drug delivery. For this reason, we believe that filling the pipeline with a larger supply of

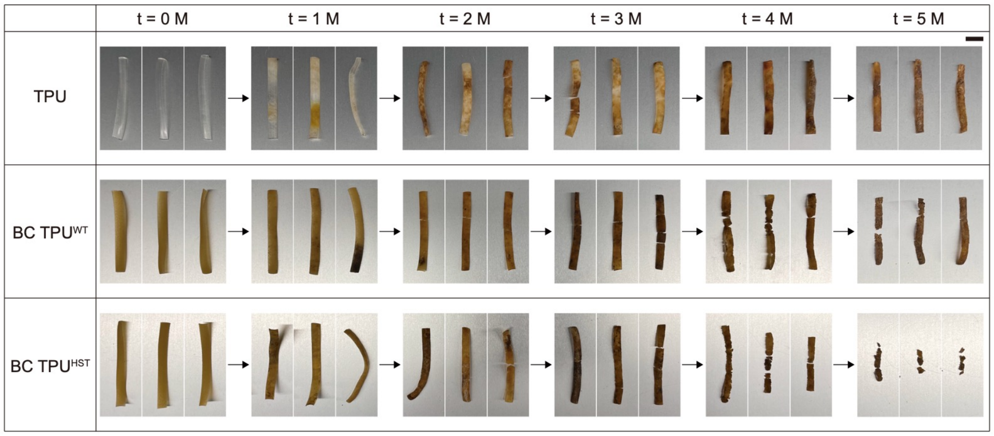


Figure 9-20: Visual changes of the disintegration of TPU and the biocomposites (BC TPUs) of *B. subtilis* and TPU, separately with wild-type *B. subtilis* and heat-shock tolerized (HST) *B. subtilis*. The experiments were over five months of incubation in autoclaved compost (37 °C with 45â€“55 % relative humidity); scale bar: 10 mm [34].

new biocomposite materials justifies an invigorated “push” towards materials innovation for non-medical applications and is needed to power translational opportunities. In this case, we not only recommend watching for signposts of accelerating scientific momentum, but partnering with agencies that fund basic science research such as the NSF Division of Materials Research and Engineering Directorate, and the DOE Office of Science to help build momentum in the development of living biocomposites.

9.2 Intermetallic and High Entropy Alloys

9.2.1 Materials for extreme conditions: Example of oxide dispersion strengthened (ODS) alloys

Materials for extreme conditions have been the focus of numerous workshops and initiatives, as, for example, in ARPA-E's ULTIMATE program `https://arpa-e.energy.gov/technologies/programs/ultimate`. Although this need often evokes extreme temperatures as found in gas turbine engines or hypersonics, there are many other stimuli such as pressure, corrosive and biological environments that represent challenges for materials development.

As an example, ODS alloys have long been touted as a class of metallics that extend the envelope of what is possible in properties for materials in extreme conditions. Most notably, they have been demonstrated to have useful properties with respect to radiation damage resistance because the presence of finely dispersed oxide particles substantially increases the specific interfacial area that acts as both a sink for point defects and as a site for recombination of, say, interstitials and vacancies [23]. Corrosion is another target of opportunity where the particle dispersion refines the microstructure via stabilization of the grain structure [88], and thereby minimizes the self-localization tendency of corrosion. The ODS approach has also been used for copper alloys where high electrical conductivity demands minimal solute levels in the matrix, [89].

Processing of ODS alloys has, however, been the Achilles heel of this class of metallics and, more specifically, the difficulties in scale-up. Most ODS alloys are made by ball-milling powders of the base alloy with finer powders of the desired oxide addition. Ball milling means placing the powders in a jar (of robust construction) along with balls made from a material of substantially higher hardness and rotating (tumbling) the jar for many hours. Such a process is self-evidently slow and not amenable to scale up.

Recently, however, progress has been reported in starting with conventionally produced metal powders and coating them with – generally – much finer oxide particles [61]. So if the metal particles have a median size of 50 microns, the oxide particles might have a median size $1000X$ smaller, i.e., 50 nm. In the cited report, it proved possible to use laser powder bed fusion (3D printing) to make bulk material, test the mechanical properties and demonstrate superior strength at temperatures above 800 $^{\circ}C$. This processing route thus side-steps the hard-to-scale sequence of ball milling followed by powder compaction and opens up the possibility of near net-shape parts. This is a promising beginning, but far more work needs to be done to evaluate the properties (particularly as a function of processing conditions) of these 3D-printed materials.

9.2.2 Materials for Extreme Conditions: Example of Intermetallics

Intermetallics as a class of materials have attracted research over many decades because of their potential for use under extreme conditions. The original interest arose from nickel-based superalloys in which it was discovered that the γ' Ni_3Al intermetallic imparts superior high temperature strength through the complex way in which dislocations interact with precipitate particles. In a certain sense, the deployment of gamma-titanium aluminide (γ -TiAl) with the application to fan blades in the compressor section of gas turbine aero-engines represents a notable success for the development of intermetallics. There are counter-examples of attempts to mature specific compounds such as $MoSi_2$ that have had minimal impact despite decades of research; as summarized by Tapia-López [65], there is the traditional use of the material in heating elements along with increasing use of $MoSi_2$-based coatings. The “Achilles heel” for this intermetallic is the so-called *pest* phenomenon in which heating (in air) through an intermediate temperature range 400 – 600 °C results in rapid oxidation and loss of integrity. In short, the dominant target application has been high temperature mechanical strength.

In recent times, however, a broader range of applications has been explored such as radiation damage resistance, catalyst particles, battery materials and specialized extraction of materials. Of these, the last two are clearly in the remit of the Dept. of Energy and unlikely to be suitable targets of opportunity for TIP. Radiation damage resistance is a specialized topic and again of more direct interest to nuclear energy, *i.e.,* Dept. of Energy. That leaves (heterogeneous) catalysis for multiple potential reactions, including de-hydrogenation of propane [45] and electrocatalytic water-splitting [84]. It appears that most of the activity has been in the vein of materials discovery so that, if industry partners could be found to provide the “pull” towards deployment by defining one or more credible applications, this might become a candidate for TIP investment.

In summary JASON recommends monitoring developments in this area that lead to commercialization.

This Page Intentionally Left Blank

10 CONCLUDING REMARKS

In summary, TIP is on a path toward translation of advanced materials via existing directorate-wide efforts within NSF. We believe that efforts targeted specifically at the key technology area of advanced materials will be fruitful, particularly if focused on materials that are currently in a *goldilocks* zone where there is both a recent push from materials innovation and a pull towards specific application spaces (Task 3 from Section 2.2). Within this document, we outlined three specific opportunities in this zone:

1. A Circular Economy for Plastics
2. Thermal and Packaging Challenges in Electronic Systems
3. Alternatives to Fluorinated Compounds in Materials for National and Economic Security Applications

Item 1 is specifically an area where there have been recent advances in the materials science research arena so it could be construed as a "Materials-Up" driver (Task 1 from Section 2.2). Items 2-3 are areas in which there is a pressing, motivating application need resulting in an "Applications-Down" perspective (Task 2 from Section 2.2). Similarly Items 2-3 are both areas in which an AI/ML approach may accelerate innovation and translation if the right data sets are obtained on which to translate these models (Task 4 from Section 2.2).

This Page Intentionally Left Blank

References

[1] U. S. Department of Defense Offices of the Assistant Secretary of Defense for Energy, Installations, and Environment and the Assistant Secretary of Defense for Industrial Base Policy. Report on critical per- and polyfluoroalkyl substance uses. `https://www.acq.osd.mil/eie/eer/ecc/pfas/docs/reports/Report-on-Critical-PFAS-Substance-Uses.pdf`, 2023.

[2] 3M Company. 3M settlement with public water suppliers to address PFAS in drinking water receives final court approval. https://investors.3m.com/news-events/press-releases/detail/1836/3m-settlement-with-public-water-suppliers-to-address-pfas.

[3] 3M Company. 3M to exit PFAS manufacturing by the end of 2025. `https://news.3m.com/2022-12-20-3M-to-Exit-PFAS-Manufacturing-by-the-End-of-2025`, 2024.

[4] ai.gov. AI Aspirations: R&D for Public Missions — ai.gov. `https://ai.gov/aspirations/`, . [Accessed 26-07-2024].

[5] ai.gov. An AI aspiration for sustainable materials. `https://ai.gov/wp-content/uploads/2024/06/AIA-Materials-0624.pdf`, . [Accessed 01-09-2024].

[6] B. Ameduri, J. Sales, and M. Schlipf. Developments in fluoropolymer manufacturing technology to remove intentional use of pfas as polymerization aids. *IRCL*, 6:18, 2023.

[7] M. Ateia, J. V. Buren, W. Barrett, T. Martin, and G. G. Back. Sunrise of pfas replacements: A perspective on fluorine-free foams. *ACS sustainable chemistry & engineering*, 11(21):7986–7996, 2023.

[8] G. T. Beckham, R. D. Allen, R. M. Baldwin, M. Reed, J. Rorrer, Y. Roman-Leshkov, J. E. McGeehan, and E. Y.-X. Chen. Transforming the science and technology of plastics recycling.

Technical report, National Renewable Energy Lab.(NREL), Golden, CO (United States), 2021.

[9] A. F. Benning. Fluorinated aliphatic phosphates as emulsifying agents for aqueous polymerizations, July 10 1951. US Patent 2,559,749.

[10] K. L. Berry. Aqueous colloidal dispersions of polymers, July 10 1951. US Patent 2,559,752.

[11] A. Bohre, P. R. Jadhao, K. Tripathi, K. K. Pant, B. Likozar, and B. Saha. Chemical recycling processes of waste polyethylene terephthalate using solid catalysts. *ChemSusChem*, 16(14): e202300142, 2023.

[12] R. C. Buck, S. H. Korzeniowski, E. Laganis, and F. Adamsky. Identification and classification of commercially relevant per-and poly-fluoroalkyl substances (pfas). *Integrated environmental assessment and management*, 17(5):1045–1055, 2021.

[13] I. R. Campbell, M.-Y. Lin, H. Iyer, M. Parker, J. L. Fredricks, K. Liao, A. M. Jimenez, P. Grandgeorge, and E. Roumeli. Progress in Sustainable Polymers from Biological Matter. *Annual Review of Materials Research*, 53(Volume 53, 2023):81–104, 2023. ISSN 1545-4118. doi: https://doi.org/10.1146/annurev-matsci-080921-083655. URL `https://www.annualreviews.org/content/journals/10.1146/annurev-matsci-080921-083655`. Publisher: Annual Reviews Type: Journal Article.

[14] Chemours. Ensuring continued supply in the face of an evolving regulatory landscape. `https://www.viton.com/en/products/apa-fluoroelastomers`, 2023.

[15] G. W. Coates and Y. D. Getzler. Chemical recycling to monomer for an ideal, circular polymer economy. *Nature Reviews Materials*, 5(7): 501–516, 2020.

[16] B. Coller and R. Califf. Traversing the valley of death: A guide to assessing prospects for translational success. *Sci. Trans. Medicine*, 1: 1–5, 2009.

[17] P. County. per-and-polyfluoroalkyl-substances-PFAS. Jul 2024.

[18] N. De Belie, E. Gruyaert, A. Al-Tabbaa, P. Antonaci, C. Baera, D. Bajare, A. Darquennes, R. Davies, L. Ferrara, T. Jefferson, et al. A review of self-healing concrete for damage management of structures. *Advanced materials interfaces*, 5(17):1800074, 2018.

[19] J. DeSimone, Z. Guan, and C. Elsbernd. Synthesis of fluoropolymers in supercritical carbon dioxide. *Science*, 257(5072):945–947, 1992.

[20] J. Elliott, M. Lebon, and A. Robinson. Optimising integrated heat spreaders with distributed heat transfer coefficients: A case study for cpu cooling. *Case Studies in Thermal Engineering*, 38:102354, 2022.

[21] M. Eminizer, S. Tabrisky, A. Sharifzadeh, C. DiMarco, J. Diamond, K. Ramesh, T. Hufnagel, T. McQueen, and D. Elbert. Openmsistream: A python package for integration of streaming data in diverse laboratory environments. *Journal of Open Scientific Software*, 8(83), 2023. `https://github.com/openmsi/openmsistream`.

[22] Environmental Working Group. Many companies market alternatives for products that contain PFAS. `https://www.ewg.org/withoutintentionallyaddedpfaspfc`, Jan 2024.

[23] T. Fu, K. Cui, Y. Zhang, J. Wang, F. Shen, L. Yu, J. Qie, et al. Oxidation protection of tungsten alloys for nuclear fusion applications: A comprehensive review. *Journal of Alloys and Compounds*, 884:161057, 2021.

[24] L. G. Gaines. Historical and current usage of per-and polyfluoroalkyl substances (pfas): A literature review. *American Journal of Industrial Medicine*, 66(5):353–378, 2023.

[25] L. M. Ghiringhelli, C. Carbogno, S. Levchenko, F. Mohamed, G. Huhs, M. Lüders, M. Oliveira, and M. Scheffler. Towards efficient data exchange and sharing for big-data driven materials science: metadata and data formats. *npj Computational Materials*, 3(1):46, 2017. doi: 10.1038/s41524-017-0048-5. URL `https://doi.org/10.1038/s41524-017-0048-5`.

[26] J. Glüge, R. London, I. T. Cousins, J. DeWitt, G. Goldenman, D. Herzke, R. Lohmann, M. Miller, C. A. Ng, S. Patton, et al. Information requirements under the essential-use concept: Pfas case studies. *Environmental science & technology*, 56(10):6232–6242, 2021.

[27] L. Gonález, N. Mukhitov, and C. Voigt. Resilient living materials built by printing bacterial spores. *Nat. Chem. Biol.*, 16:126–133, 2020.

[28] Graphene Flagship. Grapheneflagship. `https://graphene-flagship.eu/`, 2024.

[29] Z.-L. . H. J. Gregoire, J.M. Combinatorial synthesis for ai-driven materials discovery. *Nat. Synth*, 2:493–504, 2023.

[30] G. Harbeke. Optical properties of GaN. *RCA Review: A Technical Journal*, 36:163, 1975.

[31] IEEE Electronics Packaging Society. Heterogenerous Inetgration Roadmap — eps.ieee.org. `https://eps.ieee.org/technology/heterogeneous-integration-roadmap.html`. [Accessed 30-07-2024].

[32] Intel Company. Homegrown AI tools shorten design cycles to hours. `https://www.intel.com/content/www/us/en/newsroom/news/homegrown-ai-tools-shorten-design-cycles-to-hours.html#gs.d5qb8`.

[33] JASON Group. JSR-23-03 Expanding the Materials Genome

Initiative and Computational Capabilities across the DoD (MGI). 2023.

[34] H. Kim, M. Noh, E. White, M. Kandefer, A. Wright, D. Datta, H. Lim, E.Smiggs, J. Locklin, M. Rahman, A. Feist, and J. Pokorski. Biocomposite thermoplastic polyurethanes containing evolved bacterial spores as living fillers to facilitate polymer disintegration. *Nature Communications*, 15:3338, 2024.

[35] D. Kramer. Europe's experiment in funding graphene research is paying off. *Physics Today*, 74(8):20–24, 2021.

[36] T. Kwon, H. Jeong, M. Kim, S. Jung, and I. Ro. Catalytic Approaches to Tackle Mixed Plastic Waste Challenges: A Review. *Langmuir*, 40(33):17212–17238, 2024. doi: 10.1021/acs.langmuir.4c01303. URL `https://doi.org/10.1021/acs.langmuir.4c01303`. _eprint: https://doi.org/10.1021/acs.langmuir.4c01303.

[37] P. LaBeaume, K. Hernandez, E. Vitaku, T. Marangoni, E. Aqad, M. Li, C. Hoelzel, J. Lachowski, M. Hayes, S. Wong, J. Li, A. Kwok, W. Huang, J. Park, H. He, H. Mackay, C. Liu, J. Cameron, C. Xu, Q. Xie, and K. Petrillo. Disruptive non-fluorinated photoacid generators using computational chemistry and library design. In D. Guerrero and G. R. Amblard, editors, *Advances in Patterning Materials and Processes XLI*, volume 12957, page 129572B. SPIE, 2024. doi: 10.1117/12.3025297. URL `https://doi.org/10.1117/12.3025297`. Backup Publisher: International Society for Optics and Photonics.

[38] J. H. Lau. Recent advances and trends in advanced packaging. *IEEE Transactions on Components, Packaging and Manufacturing Technology*, 12(2):228–252, 2022.

[39] D. Lay, I. Keyt, S. Tiscione, and J. Kreissig. Check your tech: A guide to PFAS in electronics. https://chemsec.org/reports/check-your-tech-a-guide-to-pfas-in-electronics/, 2020.

[40] H. Li, H. A. Aguirre-Villegas, R. D. Allen, X. Bai, C. H. Benson, G. T. Beckham, S. L. Bradshaw, J. L. Brown, R. C. Brown, V. S. Cecon, J. B. Curley, G. W. Curtzwiler, S. Dong, S. Gaddameedi, J. E. García, I. Hermans, M. S. Kim, J. Ma, L. O. Mark, M. Mavrikakis, O. O. Olafasakin, T. A. Osswald, K. G. Papanikolaou, H. Radhakrishnan, M. A. S. Castillo, K. L. Sánchez-Rivera, K. N. Tumu, R. C. V. Lehn, K. L. Vorst, M. M. Wright, J. Wu, V. M. Zavala, P. Zhou, and G. W. Huber. Expanding plastics recycling technologies: chemical aspects, technology status and challenges. *Green Chem.*, 24:8899–9002, 2022.

[41] T.-S. Lin, C. W. Coley, H. Mochigase, H. K. Beech, W. Wang, Z. Wang, E. Woods, S. L. Craig, J. A. Johnson, J. A. Kalow, K. F. Jensen, and B. D. Olsen. BigSMILES: A Structurally-Based Line Notation for Describing Macromolecules. *ACS Central Science*, 5(9): 1523–1531, 2019. doi: 10.1021/acscentsci.9b00476. URL `https://doi.org/10.1021/acscentsci.9b00476`. _eprint: https://doi.org/10.1021/acscentsci.9b00476.

[42] M. Malakoutian, D. E. Field, N. J. Hines, S. Pasayat, S. Graham, M. Kuball, and S. Chowdhury. Record-low thermal boundary resistance between diamond and gan-on-sic for enabling radiofrequency device cooling. *ACS Applied Materials & Interfaces*, 13(50):60553–60560, 2021.

[43] M. B. Mitchel and W. G. Henry. Concentration of aqueous colloidal dispersions of polytetrafluoroethylene, June 5 1962. US Patent 3,037,953.

[44] M. Mulukutla, A. N. Person, S. Voigt, L. Kuettner, B. Kappes, D. Khatamsaz, R. Robinson, D. S. Mula, W. Xu, D. Lewis, H. Eoh, K. Xiao, H. Wang, J. S. Saini, R. Mahat, T. Hastings, M. Skokan, V. Attari, M. Elverud, J. D. Paramore, B. Butler, K. Vecchio, S. R. Kalidindi, D. Allaire, I. Karaman, E. L. Thomas, G. Pharr, A. Srivastava, and R. Arroyave. Illustrating an effective workflow for accelerated materials discovery. *INTEGRATING MATERIALS*

AND MANUFACTURING INNOVATION, 2024 JUN 3 2024. ISSN 2193-9764. doi: 10.1007/s40192-024-00357-3.

[45] Y. Nakaya, E. Hayashida, H. Asakura, S. Takakusagi, S. Yasumura, K.-i. Shimizu, and S. Furukawa. High-entropy intermetallics serve ultrastable single-atom pt for propane dehydrogenation. *Journal of the American Chemical Society*, 144(35):15944–15953, 2022. doi: 10.1021/jacs.2c01200. URL `https://doi.org/10.1021/jacs.2c01200`. PMID: 35984749.

[46] M. Nascimento. Brief history of the flat glass patent – sixty years of the float process. *World Patent Information*, 38:50–56, 2014.

[47] National Academies of Sciences and Division on Engineering and Physical Sciences and Board on Energy and Environmental Systems and Committee on Assessment of Solid-State Lighting and Phase. *Assessment of Solid-State Lighting, Phase Two*. National Academies Press, 2017.

[48] National Research Council and Division on Engineering and Physical Sciences and Board on Manufacturing and Engineering Design and National Materials Advisory Board and Committee on Accelerating Technology Transition. Accelerating technology transition: bridging the valley of death for materials and processes in defense systems, 2004.

[49] S. Nicholson, J. Rorrer, A. Singh, M. Konev, N. Rorrer, A. Carpenter, A. Jacobsen, Y. Román-Leshkov, , and G. T. Beckham. The critical role of process analysis in chemical recycling and upcycling of waste plastics. *Annu. Rev. Chem. Biomol. Eng.*, 13: 301–324, 2022.

[50] C. K. Ober, F. Käfer, and J. Deng. Review of essential use of fluorochemicals in lithographic patterning and semiconductor processing. *Journal of Micro/Nanopatterning, Materials, and Metrology*, 21(1):010901–010901, 2022.

[51] A. J. O'Lenick Jr. Silicones—basic chemistry and selected applications. *Journal of Surfactants and Detergents*, 3(2):229–236, 2000.

[52] Organisation for Economic Co-operation and Development. *Global Plastics Outlook*. 2022. doi: https://doi.org/https://doi.org/10.1787/de747aef-en.

[53] P. Patel. Mighty MXenes are ready for launch. 102(9), mar 2024. Publisher: Chemical and Engineering News.

[54] K. Ragaert, L. Delva, and K. Van Geem. Mechanical and chemical recycling of solid plastic waste. *Waste management*, 69:24–58, 2017.

[55] Rapid-HI. Rapid Heterogeneous Integration (Rapid-HI) Design Institute. =https://engineering.purdue.edu/Rapid-HI.

[56] L. Rivera-Tarazona, T. Shukla, K. Singh, A. Gaharwar, Z. Campbell, and T. Ware. 4d printing of engineered living materials. *Adv. Funct. Mater.*, 32:2106843, 2022.

[57] A. Rodrigo-Navarro, S. Sankaran, M. J. Dalby, A. del Campo, and M. Salmeron-Sanchez. Engineered living biomaterials. *Nature Reviews Materials*, 6(12):1175–1190, 2021.

[58] semiconductors.org. Background on semiconductor manufacturing and PFAS. `https://www.semiconductors.org/wp-content/uploads/2023/05/FINAL-PFAS-Consortium-Background-Paper.pdf`. [Accessed 26-07-2024].

[59] A. J. Shapiro, R. M. O'Dea, S. C. Li, J. C. Ajah, G. F. Bass, and T. H. Epps III. Engineering innovations, challenges, and opportunities for lignocellulosic biorefineries: leveraging biobased polymer production. *Annual review of chemical and biomolecular engineering*, 14(1):109–140, 2023.

[60] R. L. Smith, S. Takkellapati, and R. C. Riegerix. Recycling of plastics in the united states: plastic material flows and polyethylene

terephthalate (pet) recycling processes. *ACS sustainable chemistry & engineering*, 10(6):2084–2096, 2022.

[61] T. M. Smith, C. A. Kantzos, N. A. Zarkevich, B. J. Harder, M. Heczko, P. R. Gradl, A. C. Thompson, M. J. Mills, T. P. Gabb, and J. W. Lawson. A 3d printable alloy designed for extreme environments. *Nature*, 2023. doi: 10.1038/s41586-023-05893-0. URL `https://doi.org/10.1038/s41586-023-05893-0`.

[62] J. Sun, J. Dong, L. Gao, Y.-Q. Zhao, H. Moon, and S. L. Scott. Catalytic Upcycling of Polyolefins. *Chemical Reviews*, 124(16): 9457–9579, 2024. doi: 10.1021/acs.chemrev.3c00943. URL `https://doi.org/10.1021/acs.chemrev.3c00943`. _eprint: https://doi.org/10.1021/acs.chemrev.3c00943.

[63] R. Swaminathan. The next frontier: Enabling moore's law using heterogeneous integration. *Chip Scale Review*, pages 11–22, 2022.

[64] G. Tang, B. J. Gould, A. Ngowe, and A. D. Rollett. An updated index including toughness for hot-cracking susceptibility. *METALLURGICAL AND MATERIALS TRANSACTIONS A-PHYSICAL METALLURGY AND MATERIALS SCIENCE*, 53 (4):1486–1498, 2022 APR 2022. ISSN 1073-5623. doi: 10.1007/s11661-022-06612-6.

[65] J. Tapia-López, M. I. Pech-Canul, and H. M. García. Processing, microstructure, properties, and applications of mosi2-containing composites: a review. *Frontiers in Materials*, 10:1165245, 2023. ISSN 2296-8016. doi: 10.3389/fmats.2023.1165245. URL `https://www.frontiersin.org/journals/materials/articles/10.3389/fmats.2023.1165245`.

[66] The Materials Genome Initiative, U. S. multi-federal agency initiative. Materials genome initiative. `https://www.mgi.gov`, 2023.

[67] The Materials Project, Lawrence Berkeley National Laboratories. Harnessing the power of supercomputing and state of the art

electronic structure methods.
`https://legacy.materialsproject.org`, 2024.

[68] J. Tsao, S. Chowdhury, M. Hollis, D. Jena, N. Johnson, K. Jones, R. Kaplar, S. Rajan, C. Van de Walle, E. Bellotti, et al. Ultrawide-bandgap semiconductors: research opportunities and challenges. *Advanced Electronic Materials*, 4(1):1600501, 2018.

[69] A. H. Tullo. How fluoropolymer makers are trying to hold on to their business, Mar 2023. URL `https://cen.acs.org/materials/polymers/fluoropolymer-makers-trying-hold-business/101/i8`.

[70] U. S. Defense Advanced Research Projects Agency. Cranking the power on radar capabilities. `https://www.darpa.mil/news-events/2022-11-23`.

[71] U. S. Department of Energy. Solid State Lighting Program. `https://www.energy.gov/eere/ssl/solid-state-lighting`, .

[72] U. S. Department of Energy. What are critical materials and critical minerals. `https://www.energy.gov/cmm/what-are-critical-materials-and-critical-minerals`, . [Accessed 26-07-2024].

[73] U. S. Department of Energy. The history of the light bulb. `https://www.energy.gov/articles/history-light-bulb`, 2024. [Accessed 01-08-2024].

[74] U. S. Environmental Protection Agency. Per- and Polyfluoroalkyl Substances (PFAS) — US EPA — epa.gov. `https://www.epa.gov/sdwa/and-polyfluoroalkyl-substances-pfas`, 2024. [Accessed 25-07-2024].

[75] U. S. National Science and Technology Council, Office of Science and Technology Policy. Per- and Polyfluoroalkyl Substances (PFAS) report. `https://www.whitehouse.gov/wp-content/uploads/2023/03/OSTP-March-2023-PFAS-Report.pdf`, Mar 2023.

[76] U. S. National Science Foundation. Partnerships for innovation (pfi) program. `https://new.nsf.gov/funding/opportunities/partnerships-innovation-pfi`. [Accessed 01-08-2024].

[77] U. S. National Science Foundation. Convergence Accelerator Portfolio — new.nsf.gov. `https://new.nsf.gov/funding/initiatives/convergence-accelerator/portfolio`. [Accessed 26-07-2024].

[78] U. S. National Science Foundation. NSF announces nearly $50 million partnership with Ericsson, IBM, Intel, and Samsung to support the future of semiconductor design and manufacturing. `https://new.nsf.gov/news/nsf-announces-nearly-50-million-partnership`, 2023.

[79] U. S. National Science Foundation. NSF invests up to nearly $52m to align science and technology research and development investments with outcomes essential to U. S. competitiveness. `https://new.nsf.gov/tip/updates/nsf-invests-nearly-52m-align-science-technology?utm_medium=email&utm_source=govdelivery`, 2024. [Accessed 30-07-2024].

[80] U. S. National Science Foundation. NSF proposal & award policies & procedures guide (pappg). `https://new.nsf.gov/policies/pappg`, 2024.

[81] U. S. Senate. Energy act of 2020. `https://www.energy.senate.gov/services/files/32B4E9F4-F13A-44F6-A0CA-E10B3392D47A`, 2020. [Accessed 26-07-2024].

[82] U.S. National Science Foundation. Tip roadmap. `https://nsf-gov-resources.nsf.gov/files/TIPRoadmap_WEB.pdf`, 2024.

[83] D. Walsh, W. Zou, L. Schneider, R. Mello, M. Deagen, J. Mysona, T.-S. Lin, J. de Pablo, K. Jensen, D. Audus, and et al. Cript: A

scalable polymer material data structure. *ChemRxiv*, 2022. doi: 10.26434/chemrxiv-2022-xpz37.

[84] C. Walter, P. W. Menezes, and M. Driess. Perspective on intermetallics towards efficient electrocatalytic water-splitting. *Chem. Sci.*, 12:8603–8631, 2021. doi: 10.1039/D1SC01901E. URL `http://dx.doi.org/10.1039/D1SC01901E`.

[85] J. Wei, J. Liu, W. Zeng, Z. Dong, J. Song, S. Liu, and G. Liu. Catalytic hydroconversion processes for upcycling plastic waste to fuels and chemicals. *Catal. Sci. Technol.*, 13(5):1258–1280, 2023. doi: 10.1039/D2CY01886A. URL `http://dx.doi.org/10.1039/D2CY01886A`. Publisher: The Royal Society of Chemistry.

[86] M. D. Wilkinson, M. Dumontier, I. J. Aalbersberg, G. Appleton, M. Axton, A. Baak, N. Blomberg, J.-W. Boiten, L. B. da Silva Santos, P. E. Bourne, J. Bouwman, A. J. Brookes, T. Clark, M. Crosas, I. Dillo, O. Dumon, S. Edmunds, C. T. Evelo, R. Finkers, A. Gonzalez-Beltran, A. J. G. Gray, P. Groth, C. Goble, J. S. Grethe, J. Heringa, P. A. C. 't Hoen, R. Hooft, T. Kuhn, R. Kok, J. Kok, S. J. Lusher, M. E. Martone, A. Mons, A. L. Packer, B. Persson, P. Rocca-Serra, M. Roos, R. van Schaik, S.-A. Sansone, E. Schultes, T. Sengstag, T. Slater, G. Strawn, M. A. Swertz, M. Thompson, J. van der Lei, E. van Mulligen, J. Velterop, A. Waagmeester, P. Wittenburg, K. Wolstencroft, J. Zhao, and B. Mons. The fair guiding principles for scientific data management and stewardship. *Scientific Data*, 3(1):160018, 2016. doi: 10.1038/sdata.2016.18. URL `https://doi.org/10.1038/sdata.2016.18`.

[87] Y. Xiao, L. J. Miara, Y. Wang, and G. Ceder. Computational screening of cathode coatings for solid-state batteries. *Joule*, 3(5): 1252–1275, 2019. ISSN 2542-4351. doi: https://doi.org/10.1016/j.joule.2019.02.006. URL `https://www.sciencedirect.com/science/article/pii/S2542435119300868`.

[88] J. Xie, J. Zhang, Z. You, S. Liu, K. Guan, R. Wu, J. Wang, and J. Feng. Towards developing mg alloys with simultaneously improved strength and corrosion resistance via re alloying. *Journal of Magnesium and Alloys*, 9(1):41–56, 2021.

[89] H. Yang, Z. Ma, C. Lei, L. Meng, Y. Fang, J. Liu, and H. Wang. High strength and high conductivity cu alloys: A review. *Science China Technological Sciences*, 63(12):2505–2517, 2020.

[90] S. Yoshida, K. Hiraga, T. Takehana, I. Taniguchi, H. Yamaji, Y. Maeda, K. Toyohara, K. Miyamoto, Y. Kimura, and K. Oda. A bacterium that degrades and assimilates poly (ethylene terephthalate). *Science*, 351(6278):1196–1199, 2016.

[91] S. Zhang, Z. Li, H. Zhou, R. Li, S. Wang, K.-W. Paik, and P. He. Challenges and recent prospectives of 3d heterogeneous integration. *E-Prime-Advances in Electrical Engineering, Electronics and Energy*, 2:100052, 2022.

This Page Intentionally Left Blank

A APPENDIX: Summary of Findings and Recommendations

A.1 Listing of Findings

Finding 2.1: Technology integration requires that materials demonstrate a value proposition (economic, life cycle, regulatory) and be scalable, reliable, and durable.

Finding 2.2: High impact translational opportunities for TIP investment in advanced materials are to be found in a "goldilocks zone" where there is both a *push* from a recent materials or materials system discovery and a *pull* from an existing or new application or technology space in which that material provides unique advantages and presents a value proposition. (**F1**)[15]

Finding 3.1: Common barriers prevent new materials and materials processing techniques from translating into new technologies. Particularly challenging are issues associated with scaling up from the gram scale typical of bench-top work in academic labs to the multi-kilogram scale needed for development of materials prior to further scale-up in a pilot plant or manufacturing facility. This "development scale" highlights new challenges in materials synthesis, scale-up, and processing. The solutions to these challenges are iterative with basic science and lead to further innovation. (**F2**)

Finding 3.2: Key approaches to counter these common barriers to translation include (**F3**):

---

[15] designation **F1** indicates this is a Key Finding or Recommendation included in the Executive Summary of this report

a) Scaling up beyond lab-scale synthesis

b) Early system-level integration of new materials

c) Uniform testing and understanding of performance metrics, including durability and reliability

d) Early inclusion of detailed technoeconomic and lifecycle analyses

e) Engaging with industrial partners and government regulators

Finding 4.1: Accessible facilities that enable expansion beyond laboratory-scale experiments and models are essential for addressing scale-up challenges. These facilities amplify investments by engaging more researchers than can be directly funded, enhancing uniformity in testing and materials reliability, and broadening workforce development. (**F4**)

Finding 5.1: AI/ML could play a substantial, increased role in accelerating the creation of new materials with specific desired characteristics. Rather than mapping such opportunities to "specific classes of materials," JASON believes that the opportunities need to leverage and are critically dependent on gathering and analyzing large-scale data of basic materials properties, details of processing and manufacturing, as well as performance within the final applications. Although details of AI/ML will differ according to material and application, the collection and calibration of such data will be facilitated by (**F5**):

1. Collaborations with existing national user facilities
2. Establishing specialized user facilities as needed for specific materials problems
3. Instrumented automation of experiments and scale-up

4. Capturing, labeling, and categorizing large amounts of curated process data
5. Uniformity in testing and characterization
6. Working with industrial experts able to help define and populate relevant data bases

Finding 6.1: Significant federal and industrial funding has led to the development of numerous possible routes towards a circular economy for plastics use and enabled inventions ranging from new catalysts for chemical recycling to new biomass derived materials. So far, commercialization has been limited to relatively small start-up-scale efforts (**F6**).

Finding 6.2: Laboratory experiments are performed at small scale on pure materials, while full-scale production requires integration with accepted processing techniques for less ideal polymers. Similarly, biomass processing experiments at the lab scale use a single feedstock, but accurate life-cycle analyses (LCA) and technoeconomic analyses (TEA) require the use of realistic feedstocks and appropriately scaled synthesis and processing (**F8**).

Finding 6.3: Scale-up from a round bottom flask or a Parr reactor in a laboratory to process-scale equipment handling highly viscous polymer melts is an iterative process that presents new challenges but can also inspire new scientific directions. This iterative process is not generally pursued via basic science programs in polymer science and the lack of iterative understanding, as well as the lack of universal rules to scale-up to larger process equipment and production rates, are major barriers towards the translation of new polymer recycling solutions (**F9**).

Finding 6.4: While basic science discoveries are performed at small scale on pure materials, translational activity is needed to translate these discoveries to processing techniques appropriate for large-scale, highly viscous, poorly soluble, chemically impure commodity plastics.

Finding 6.5: In order to find market translation, biomass derived polymers must both have properties equal to or better than current plastics and have demonstrated inexpensive synthetic routes that are robust to variations in feedstock. Testing of processibility and durability requires a much larger scale of materials (¿¿kilogram) as well as equipment and safety practices unusual in academic settings.

Finding 6.6: Life cycle analysis (LCA), encompassing materials, energy and water costs, environmental impacts, and technoeconomic analysis (TEA), encompassing a true comparison to the cost of existing technologies, are critical to a compelling value proposition. The LCA and TEA estimations improve as science and process design mature (**F7**).

Finding 7.1: Advances in modern high-performance electronics depend on more than scaling to smaller feature sizes and higher densities. Innovative 2.5D and 3D device architectures composed of multiple chips and chiplets, e.g., Heterogeneously Integrated (HI) Systems in a Package (SiP), will be critical for future advanced computing. These architectures will require new materials solutions for thermal management and packaging (**F10**).

Finding 7.2: High power electronics generate large heat fluxes at the die level. Academic and small research laboratories have introduced materials with thermal conductivities above 300 W/mK as heat spreaders, including AlN, BAs, and diamond into such devices. Interfacial engineering has enabled the advancement of the integration and performance of these technologies. However, these are not all integrated through scalable manufacturing methods and limit the transition of this solution to high power/high heat flux electronics.

Finding 7.3: New materials are needed to reduce thermal interface resistance and thermomechanical stresses within packaged electronics. Materials may include carbon nanomaterials, metal interconnects, and polymer composites.

Finding 7.5: Advanced microelectronics systems (such as HI in SiPs) exacerbate challenges in thermal management, offering opportunities for new materials and material systems solutions. Thermal effects in such HI systems are strongly coupled to electrical and mechanical performance, and materials solutions for these "Thermal Interface Materials" (TIMs) must also accommodate these constraints(**F11**).

Finding 7.5: Modeling and simulation are crucial for directing materials choices and strategic testing for the thermal performance of high-performance integrated HI system. Modeling tools need to be extended to cover the full range of length scales and include thermal-electrical-mechanical effects across the numerous interfaces in these systems. Additionally, simulations must consider details of how HI systems are assembled, such as the methods of materials deposition (**F12**).

Finding 7.6: AI and ML can improve the quality of modeling and simulation of materials for thermal and interfacial management of microelecronic systems, but can only achieve this with an extensive, well-catalogued and curated database of necessary materials and process parameters, along with system-level performance data. Data collection should be explicitly structured to enable the investigation and quantification of process-structure-property relationships through AI/ML (**F13**).

Finding 7.7: For the microelectronics industry, the mismatch with the research community in timescales for translation readiness and systems-level validation is particularly acute. Industrial process details and quality-control monitoring are generally not open to the public.

Finding 8.1: The essential use concept [75] as well as the American Innovation and Manufacturing Act (AIM) protect or allow for continued use of essential products if use of a replacement substance is impossible or impractical. While these provisions address regulatory changes and allow for continued use, they cannot protect even essential uses from market constrictions that result in a loss of availability of products (**F16**).

Finding 8.2: PFAS supplies are likely to become constrained by market contractions and reduced domestic production. Market forces are already driving replacements for consumer products. The essential use concept and access to remaining supply lines will protect the immediate needs of the economic security and national security relevant applications, but the supply is now at risk, making these PFAS products *critical materials* (**F14**).

Finding 8.3: Integrated dependencies of products and PFAS materials for both the microelectronics industry and for specialized national security applications have evolved over decades of co-development. PFAS materials are now critical to economic and security applications and are in some cases essential to performance of the relevant products.

Finding 8.4: In the prior decades of research and development, a vast amount of data, much of it proprietary to industry, has been amassed on the properties and synthesis of PFAS materials, as well as alternative materials that have been considered for similar functions. While much of this may be soon leveraged for near-term solutions, in some application cases, the Carbon-Fluorine bond in PFAS may be irreplaceable because, for example, it imparts extraordinary temperature and chemical stability. (**F15**).

Finding 8.5: Several methods for alternatives to fluoropolymers or for alternative fluoropolymer manufacturing are being developed to reduce environmental leaching. Transitions to these alternatives will likely focus on large markets with less demanding requirements. Consequently, the DoD may struggle to find manufacturers for specialty versions needed for their essential use applications including binders for explosives and o-rings for demanding environments (**F17**).

Finding 8.6: As a part of the National Science Foundation, NSF-TIP has access to a broad basic research platform and is therefore ideally situated to accelerate the materials discovery and translation of PFAS alternatives needed by other agencies and missions.

Finding 8.7: The already-existing vast amount of industrial data on the properties and synthesis of PFAS materials and alternative materials can constitute a substantial and highly-leveraged data base for AI approaches that may be able to reduce time-to-translation of PFAS alternatives (**F18**).

A.2 Listing of Recommendations

Recommendation 2.1: NSF-TIP should focus on materials maturity as defined by value proposition, scalability, durability, and reliability in identifying materials systems that are compelling research translation investments (**R1**). [16]

Recommendation 2.2: NSF-TIP should consider a set of exemplar areas which satisfy a “goldilocks zone” of materials maturity in terms of translational readiness.

---

[16] designation **R1** indicates this is a Key Finding or Recommendation included in the Executive Summary of this report

Section 6: A Circular Economy for Plastics

Section 7: Thermal and Packaging Challenges in Electronic Systems

Section 8: Replacement of Fluorinated Compounds in Formulations and Materials for Semiconductors and Energetics

Recommendation 2.3: 2-D materials ranging from graphene to MXenes have impressive properties but a unique *pull* towards a specific application or technology was not yet clear to us. There continue to be exciting developments, particularly in MXenes so we recommend a periodic survey of application or technology *pull*.

Recommendation 2.4: Ceramics and composites are important materials for national security and energy applications such as thermal barrier coatings. Outside of this already substantially funded context, we did not find discoveries that would provide a strong *push* towards translation based on new materials design paradigms or discoveries. We recommend observation for strong *pushes* towards translation in areas in which investments will not be swamped by existing investments by DOD.

Recommendation 3.1: NSF-TIP funding should focus on addressing the "beyond-lab-scale" barriers to translating materials into new technologies. This includes scaling materials production from bench-scale (subgram to gram-scale, depending on materials category) to development scale (kilogram and greater, depending on the application) and supporting necessary iterations with basic science to bridge material development toward significant applications (**R2**).

Recommendation 3.2: NSF-TIP should establish strong and diverse relationships with the entities that fund the basic science materials discovery efforts that will ultimately push translation. These include the NSF Division of Materials Research and Engineering Directorates as well as other agencies including the National Institute of Standards and Technology (**R5**).

Recommendation 3.3: Given the mandate within the CHIPS and Science Act to develop translational research and development efforts that benefit national and economic security [17], we recommend NSF-TIP establish strong relationships and communication with entities likely to *pull* new innovations. These include the Department of Defense, regulatory agencies such as the Environmental Protection Agency, the national security community, and a broad base of industrial representatives in materials technologies (**R6**).

Recommendation 4.1:: In parallel with direct R&D investments, NSF-TIP should consider funding independent facilities relevant to different materials and application areas to address common barriers to materials translation. These facilities should be established with data generation/curation and AI/ML training in mind, following best practices for uniform data handling to enable future use in AI/ML models and training (**R3**).

Recommendation 5.1: NSF-TIP advanced materials programs should be implemented with focused data generation/curation and potential AI/ML training in mind. TIP should provide each program with sufficient resources to both use and develop realistically-sized and effective data bases related to the materials goals of the program. Specific opportunities for AI/ML will be amplified in the focus areas of Thermal Management for Semiconductor Packaging and Alternatives to Fluorinated Materials in this report (**R4**).

Recommendation 6.1:. NSF-TIP should make investments in translation of plastics waste recycling specifically for the large scale consumer polyolefins (*e.g.,*polypropylenes and polyethylenes), polyvinyl

---

[17] `https://www.congress.gov/bill/117th-congress/house-bill/4346`

chloride, and polystyrene where *development scale* experiments and iterative scale-up are critical to success (**R7**).

Recommendation 6.2: NSF-TIP should support iterative process development of recycling solutions based on recent scientific breakthroughs in polymer chemical recycling, specifically, development of techniques and catalysts compatible with large scale processing of plastics likely to advance breakthroughs towards translation. Further, development of catalysts that are tolerant to the impurities and additives in commodity polymers will occur iteratively as experiments proceed at the development scale (**R8**).

Recommendation 6.3: We recommend that NSF's efforts in translating recycling and upcycling chemistries focus on specific commodity polymers which are only sparsely recycled using current technologies: polyolefins (polyethylene, polypropylene), poly(vinyl chloride), and polystyrene.

Recommendation 6.4: Specifically regarding chemical recycling approaches, NSF-TIP should focus on development of processing routes amendable to commodity plastics degradation and catalysts compatible with large-scale processing of highly viscous plastics to advance new routes of chemical recycling towards translation. Similarly, the development of enzymes and catalysts that are tolerant to the impurities and additives in commodity polymers should also be supported.

Recommendation 6.5: Create development-scale synthesis capabilities to fully demonstrate the viability of biomass derived polymers as alternatives to current commodity materials. The equipment and practices for such a level of scale-up are not typically found in academic laboratory settings. We recommend NSF-TIP consider this as part of the facilities recommended in **R3**.

Recommendation 6.6: Ensure that LCA and TEA are completed in-pace with iterative scale-up processes to give realistic feedback on the viability of plastic circularity solutions and to inspire problem solving (**R9**).

Recommendation 7.1: NSF TIP should fund the integration of high thermal conductivity heat spreaders at the die level into scalable fab-level manufacturing methods. This includes direct growth or deposition of these layers, bonding, and the tailoring of interfacial chemistry and properties to enable advanced heat spreading solutions at scale. Moreover, materials innovations and surface chemistry that can enhance heat removal through liquid cooling should also be considered.

Recommendation 7.2: NSF TIP should fund scaling and translation of thermal interface materials (TIM) informed by system requirements. These materials must bond at low temperature and can enable new topological designs.

Recommendation 7.3: NSF-TIP should fund research projects that model, process and evaluated possible TIMs within a systems context. This will lay the foundation for a long-term better match between research innovation and industrial adoption in advanced materials for microelectronics (**R10**).

Recommendation 7.4: NSF TIP, in partnership with other areas of NSF and other organizations funding basic research, should fund the development of multi-scale, multi-physics systems-level models for thermal management in HI systems, including coupled thermal-electrical-mechanical effects (**R11**).

Recommendation 7.5: NSF TIP should leverage and expand existing facilities to pilot multi-level, multi-property SiP testing for the research community, establishing well-calibrated procedures for such testing (**R12**).

Recommendation 7.6: NSF TIP should partner with other relevant government agencies to create pilot facilities for simple, but well controlled and monitored, integrated processing for HI microelectronics thermal management. These pilot facilities should collect and curate processing-related and systems-level performance data, which will enable AI/ML -facilitated system-level thermal, electrical, and mechanical models supportive of new materials integration (**R13**).

Recommendation 8.1: NSF-TIP should focus efforts on PFAS replacements that are critical to economic security, e.g., fluorine-free photo-acid generators for lithography in the microelectronics industry, and national security, e.g., DoD-specific applications, with particular attention to drop-in alternative materials to minimize disruption in essential uses (**R14**).

Recommendation 8.2: For irreplaceable fluorinated materials in essential applications, NSF-TIP should prioritize translation of manufacturing and processing methods, with highest priority on eliminating environmental release, e.g., synthesis and manufacture of fluoropolymers that do not contain leachable fluorinated small molecule surfactants. (**R15**).

Recommendation 8.3: NSF TIP should focus on translation of PFAS alternatives for application integration under use conditions (DoD, DOE-NNSA, and microelectronics) via systematic discovery, production and testing.

Recommendation 8.4: NSF TIP should support the transition from PFAS by collaborating with industry on historic data and by implementing expanded Materials Genome Initiative R&D concepts under the AI Aspiration for Sustainable Materials [4]. This work will include supporting data bases of historical and new structural [12], physical and functional properties, as well as training data for processing procedures, all of which can then be used in accelerating discovery of candidate materials and processes (**R16**).

This Page Intentionally Left Blank

B APPENDIX: Briefers to JASON

We are grateful for the introductory briefings arranged by NSF:TIP that set the context for the materials systems studied by JASON:

Topic	Name	Organization
Microelectronics and Semiconductor Packaging	David Xu	Intel
Ceramics	Don Lipkin	Texas A&M University
Sustainable Polymer Translation	David Parrillo	Dow Chemical
Translation of Polymer Materials	Joe DeSimone	Stanford University
Sustainable Materials from Biomass	Thomas Epps, III	University of Delaware
Critical Materials	Rod Eggert	Colorado School of Mines
Bioprocessing of Critical Materials	Yoshiko Fujita	Idaho National Laboratories
Composites	Raj Singh	Oklahoma State University
MXenes	Babak Anasori	Purdue University
Graphene and 2D Materials	Cary Hill	Graphene Counsil
DOD Translation of Materials	Aisha Haynes	OUSD (R&E)/S&T
Division of Materials Research at NSF	Germano Iannachionne	NSF-DMR

This Page Intentionally Left Blank

C APPENDIX: Sample Funding Scheme for a Materials Translational Opportunity: PFAS

This section relates to a funding scheme for work in replacing fluorinated compounds for applications in economic and national security applications (semiconductors and Department of Defense Applications). The scientific motivations and discussion of proposed technical directions are included in Section 8.

I. We recommend that new programs in NSF-TIP on translation for advanced materials begin with Ideas Labs for the purposes of building consensus around early phase scientific targets.

   A. As described in the 2024 NSF Grant Proposal and Award Policies and Procedure Guide, ””Ideas Lab” is a type of proposal to support the development and implementation of creative and innovative project ideas that have the potential to transform research paradigms and/or solve intractable problems. An Ideas Lab may be run independently, or in parallel, with the issuance of an NSF funding opportunity on the same topic. These project ideas typically will be high-risk/high-impact, as they represent new and unproven ideas, approaches and/or technologies” [80]

   B. In the area of fluorinated materials replacement, we recommend Ideas labs bringing together industries ranging from chemical manufacturers to end users (semiconductor manufacturers and/or defense contractors depending on the theme). We also recommend participation of agencies including DOE-NNSA, DARPA, and DoD who also represent the pull towards alternative materials. In this instance, the Ideas lab should generate information regarding the:

  i. Key areas of alternatives exploration already under consideration/development/commercial use (for example: surface coatings and photoacid generators for the semiconductor industry; alternative binders for energetics, and high temperature/high chemical stability o-rings for the defense and national security interests).
  ii. Discussion of the functional properties of these essential use materials and methods in which they are qualified.
  iii. Current knowledge base for understanding how the structure of current materials lead to their functional use with intent of driving the AI/ML discovery of alternatives.
  iv. Discussion of methodology of how efforts funded by NSF-TIP can work with DoD and DOE-NNSA to define the critical use properties and ultimate targets.

II. We recommend the Request for Proposal Structure be set in advance but allow for specific targets and collaborations that emerge from the Ideas Lab Workshops. We believe that it is crucial that the application *pull* which we have discussed within the context of Translational Opportunities be strongly represented and engaged. For this reason, we recommend that NSF partner with industry (as, for example has been done with the semiconductor in the context of the Future of Semiconductors (FuSe) initiative [78]. We recommend similar co-funding partnerships with the DoD and/or DOE-NNSA in terms of applications relevant for National Security

III. We recommend the Funding Scheme in this area match the Phase 1 and Phase 2 structure of other programs within NSF-TIP:

  A. Phase I goals should include

   i. Construction of a knowledge bank of known structure/process/function relationships
   ii. Automated exploration of parameter space for identifying promising candidates
   iii. Preliminary testing of function, environmental/health impacts
   iv. Preliminary techno-economic and lifecycle analyses of alternative materials

B. Phase II goals should include

   i. Accelerated fabrication and testing using automated procedures where possible
   ii. Accelerated scale up for best candidates identified
   iii. In depth environmental/health assessment
   iv. In depth techno-economic analysis
   v. Active effort to hand off for continuing venture support or commercial development

C. Accompanying facility support to promote:

   i. Data curation, AI and ML directed materials translation.
   ii. Mapping structure and properties among existent PFAS materials as well as new alternative materials and processes.
   iii. Partnering with PFACT Convergence Accelerator which is developing AI materials discovery models that would benefit from training on such data sets.

This Page Intentionally Left Blank

D APPENDIX: Examples of Existing Programs to Enhance Translational Opportunities

Acronym	Program	Funding Source	Description
SBIR	Small Business Innovation Research	11 Federal Agencies	Small business R&D
STTR	Small Business Technology Transfer	5 Federal Agencies	Small business/university
GOALI	Grant Opportunities for Academic Liaison with Industry	NSF-wide	University-industry collaboration
ERC	Engineering Research Center	NSF Engineering Directorate	Societal Impact
TIPS CAP	Convergence Accelerator Program	NSF Directorate for Technology Innovation and Partnerships (TIP) Directorate	Ideation and commercialization phases
STC	Science and Technology Centers	Office of Integrative Activities	Large scale, long term research and education projects
RIE	Regional Innovation Engines	TIP	Grow and sustain regional innovation

This Page Intentionally Left Blank

E APPENDIX: Promising Polymer Upcycling Catalysts

Mechanism of reaction	Catalysts	Plastics
Hydrogenolysis [62]	Metals (Pt, Ru, Ni, Co) supported on non-acidic inorganics (SiO_2, Al_2O_3, CeO_2, TiO_2, ZrO_2, C)	Polyethylene and Polypropylene
Catalytic Cracking [62]	Acids (F-Al_2O_3, SiO_2-Al_2O_3, strong Brønsted acid zeolites)	Polyethylene, Polypropylene and Polystyrene
Hydrocracking [62]	Tandem metal (Pt, Ru, Ni, Co, Mo, W) acids (F-Al_2O_3, Cl-Al_2O_3, SiO_2-Al_2O_3, strong Brønsted acid zeolites) Notable: Pt/F-Al_2O_3, $Pt/WO_3/ZrO_2$	Polyethylene and Polypropylene
Metathesis [62]	Re_2O_7/γ-Al_2O_2, CH_3ReO_3/Cl-Al_2O_3, $PtSn/\gamma$-Al_2O_3 with Re_2O_7/γ-Al_2O_3, Pt/γ-Al_2O_3 with WO_3/SiO_2	Polyethylene
Oxidation[62]	$KMnO_4$, Co(naphthenate)$_2$, Cu(stearate)$_2$, Co(acac)$_2$, MoO_3/SiO_2, Ru/TiO_2	Polyethylene and Polypropylene
Hydrogenolysis [85]	Ru or Mn complexes, MoO_x, Hf(OTf)$_4$ + Pd/C, Ru/NbO_x	Polyesters, Polycarbonates, Polyethers